

Kronecker product in terms of Hubbard operators and the Clebsch-Gordan decomposition of $SU(2) \times SU(2)$

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Abstract. We review the properties of the Kronecker (direct, or tensor) product of square matrices $A \otimes B \otimes C \cdots$ in terms of Hubbard operators. In its simplest form, a Hubbard operator $X_n^{i,j}$ can be expressed as the n -square matrix which has entry 1 in position (i, j) and zero in all other entries. The algebra and group properties of the observables that define a multipartite quantum system are notably straightforward in such a framework. In particular, we use the Kronecker product in Hubbard notation to get the Clebsch-Gordan decomposition of the product group $SU(2) \times SU(2)$. Finally, the n -dimensional irreducible representations so obtained are used to derive closed forms of the Clebsch-Gordan coefficients that rule the addition of angular momenta. Our results can be further developed in many different directions.

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1 Introduction

The Kronecker product, represented by the symbol \otimes , has attracted the attention of researchers in diverse areas of mathematics and theoretical physics over the last decades [1–9]. Introduced by Zehfuss in 1858 (see the historical review given in [4]), this is a matrix operation also known as direct or tensor product, defined for matrices $A = [a_{i,j}]$ and B of any order to be $A \otimes B = [a_{i,j}B]$. That is, for instance

$$A \otimes B = \left(\begin{array}{ccc} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{array} \right) \otimes B = \left(\begin{array}{ccc|ccc} a_{11}B & a_{12}B & a_{13}B & & & \\ & & & a_{21}B & a_{22}B & a_{23}B \end{array} \right).$$

Matrix calculus includes the derivatives of a matrix with respect to a scalar, a scalar with respect to a matrix, and a matrix with respect to a matrix; all these operations are defined in terms of the product \otimes [5–7] (other interesting applications can be found in [9]). In physics, this product arises quite naturally if the group properties of the

dynamical variables of a given system are considered [10–12], and it is fundamental in the study of multipartite systems [13, 14]. Indeed, the Clebsch-Gordan decomposition of the Kronecker product of two irreducible representations is one of the most useful problems in group theory, since the reduction of such a product into the sum of irreducible representations confirms the unicity of the representation for the simple reducible groups [15]. It is then quite natural to find immediate applications of both, the product \otimes and the Clebsch-Gordan decomposition, in the addition of angular momenta [16] as well as in the identification of symmetries in quantum physics [17].

Despite the simplicity of its definition, calculating the tensor product $A \otimes B \otimes C \otimes \dots$ becomes cumbersome for large matrix sizes and/or for a large number of factors. This fact is particularly notable in the design of fast Fourier transform algorithms where the factorization of the discrete Fourier matrix \tilde{F}_n is relevant. Namely, for $n = 2m$ with $m \in \mathbb{N}$, the n -square (Fourier) matrix¹:

$$F_n = [f_{i,j}], \quad f_{i,j} = w^{(j-1)(i-1)}, \quad i, j = 1, 2, \dots, n, \quad w = e^{2\pi i/n}, \quad (1)$$

can be expressed as the product

$$F_n = B_n(\mathbb{I}_2 \otimes F_m)\Pi_n^T,$$

where

$$B_n = \begin{pmatrix} \mathbb{I}_m & \Omega_m \\ \mathbb{I}_m & -\Omega_m \end{pmatrix}, \quad \mathbb{I}_k = \text{diag}(\underbrace{1, 1, \dots, 1}_{k\text{-times}}), \quad \Omega_k = \text{diag}(1, w, w^2, \dots, w^{k-1}),$$

and Π_k is the $k \times k$ -permutation matrix obtained by grouping the odd columns of the identity \mathbb{I}_k first, and the even columns second. Hereafter A^T is the matrix transpose of A . The procedure can be repeated if m is even. Indeed, if $n = 2^t$, $t \in \mathbb{N}$, then F_n can be factorized into the product of $t = \log_2 n$ matrix factors (Cooley-Tukey factorization):

$$F_n = (\mathbb{I}_1 \otimes B_n)(\mathbb{I}_2 \otimes B_{n/2})(\mathbb{I}_4 \otimes B_{n/4}) \cdots (\mathbb{I}_{n/2} \otimes B_2)P_n^T, \quad (2)$$

with P_n^T the bit-reversing permutation matrix [18]. Note that each factor $\mathbb{I}_k \otimes B_{n/k}$ in (2) has only two nonzero entries per row. Thus, only $2n$ of the n^2 entries associated to $\mathbb{I}_k \otimes B_{n/k}$ are different from zero. This fact suggests that there must be a better and simpler form of calculating the Kronecker product in the factorization algorithms.

On the other hand, the entries of the first row and column of the Fourier matrix (1) are all equal to unity while the other entries are either ± 1 or $\pm i$. Thus, F_n is a dephased, complex Hadamard matrix [19]. The relevance of a dephased matrix is that only its lower right $(n-1)$ -square submatrix is necessary in the calculations where it is involved. In this subject, it can be shown that the product $D_r H D_c$ brings any Hadamard matrix H into the dephased form for a pair of uniquely determined diagonal unitary matrices D_r ,

¹A Fourier matrix $\tilde{F}_n = F_n/\sqrt{n}$ is unitary. Here we also refer to (1) as Fourier matrix although it is a rescaled version of \tilde{F}_n .

and D_c [19]. The construction can be simplified since two Hadamard matrices, H_1 and H_2 , are equivalent if there exist diagonal unitary matrices D_1 and D_2 , and permutation matrices P_1 and P_2 , such that [19, 20]:

$$H_1 = D_1 P_1 H_2 P_2 D_2. \quad (3)$$

According to the former property, H_1 is dephased if $D_1 = D_r$ and $D_2 = D_c$, no matter the form of $P_1 H_2 P_2$. In this case dephasing is equivalent to the permutation of rows and columns defined by P_1 and P_2 . However, it is not easy to verify whether there exist such permutations [19]. The problem becomes even more complicated for large size matrices since the permutations grow as $N!$ Then, it is apparent the necessity of a proper framework in which the determination of the above described permutations becomes a tractable problem.

In general, the matrix algebra includes algorithms that are fairly complicated and cumbersome for either matrices of large sizes or a large number of matrices to operate with. It would therefore be desirable to construct a mathematical framework in which the problems like those aforementioned are feasible; no matter the number or the size of the matrices involved. To get a suitable approach it is useful to consider the operators $X^{p,q}$ introduced by Hubbard in 1964 [21] (see also [22]). These obey the multiplication rule

$$X^{i,j} X^{k,m} = \delta_{jk} X^{i,m}, \quad (4)$$

and have the properties

$$(X^{i,j})^\dagger = X^{j,i}, \quad \sum_k X^{k,k} = \mathbb{I}, \quad [X^{i,j}, X^{k,m}]_\pm = \delta_{jk} X^{i,m} \pm \delta_{mi} X^{k,j}, \quad (5)$$

the sublabel in $[A, B]_\pm$ stands for either the commutator $(-)$ or the anticommutator $(+)$ of A and B .

Hubbard operators provide a way to study groups of particles that interact strongly one with each other in such a way that a weak interaction between the groups is also allowed². For example, they are useful in the description of atoms in which Coulomb repulsion prevents double-occupancy of a given orbital [23]. In such cases, the strong interactions determine the energy of the groups of particles and can be included in the Hamiltonian as linear combinations of the Hubbard operators [21, 22]. This is the situation for strongly correlated electrons [24], whether they are in a cavity [25] or in a two-atom molecule [26], as well as for double quantum dots [27, 28] among other systems.

Given an n -dimensional vector space \mathcal{H}_n with orthonormal basis $\{|\psi_k\rangle\}_{k=1}^n$, the Hubbard operators are written in terms of the outer products of the basis elements:

$$X_n^{i,j} := |\psi_i\rangle\langle\psi_j|, \quad i, j = 1, 2, \dots, n. \quad (6)$$

²To distinguish between the particles of different groups, Hubbard used $X_{pq}^{(i)}$ [21] as well as X_i^{pq} [22] to denote the operator $|i, p\rangle\langle i, q|$, with i labeling a given group while $|i, p\rangle$ and $|i, q\rangle$ represent two different states of a particle in that group. In contrast, we use a sub-label “ n ” to denote the matrix order of the linear representation of the operator $X^{i,j}$, as this is done in equation (6).

That is, the operator $X_n^{i,j} = |\psi_i\rangle\langle\psi_j|$ is a representation of $X^{i,j}$ in the space \mathcal{H}_n . This causes a transition from the state $|\psi_j\rangle$ to the state $|\psi_i\rangle$ of the system that is described by the vectors in \mathcal{H}_n . In general, any linear operator $O : \mathcal{H}_n \rightarrow \mathcal{H}_n$ can be represented in terms of the Hubbard operators

$$O = \sum_{i,j} o_{i,j} X_n^{i,j}, \quad o_{i,j} = \langle\psi_i|O|\psi_j\rangle. \quad (7)$$

This property plays a central role in what follows since the operators $X_n^{i,j}$ are the cornerstone of our approach. Using the Hubbard's representation (7) one can address the algebra of square matrices in compact form, no matter the size or the number of the factors. Problems like the determination of the permutation matrices fulfilling (3) become simpler in this notation. Indeed, if the basis vector $|\psi_k\rangle$ is the n -tuple that has a unity in the k -th position and all other entries equal to zero, the Hubbard operator (6) is in its simplest form:

$$X_n^{i,j} = \begin{pmatrix} 0 & & & & & & \\ & 0_{(i-1)\times(j-1)} & & \vdots & & 0_{(i-1)\times(n-j)} & \\ & & \cdots & 0 & & & \\ 0 & & & 1 & 0 & \cdots & 0 \\ & & & 0 & & & \\ & & & \vdots & & & \\ & 0_{(n-i)\times(j-1)} & & 0 & & 0_{(n-i)\times(n-j)} & \end{pmatrix}, \quad (8)$$

where $0_{s\times t}$ is the null matrix of order $s\times t$. In other words, $X_n^{i,j}$ is the n -square matrix for which all the entries are zero except the one at the i -th row and the j -th column, where it takes the value 1. Such an array of zeros and a single unit is appropriate to operate the Kronecker products $\mathbb{I}_k \otimes B_{n/k}$ of Eq. (2) in plain notation; these products are but the linear combination of only $2n$ Hubbard operators.

This work attempts to stimulate further progress in the applications of the Hubbard operators by introducing a useful manner to calculate the Kronecker product. The paper is structured in two main parts. First, in Section 2 some basic definitions and the Hubbard notation are introduced. In Section 3 we review some of the most important properties of the direct product by using the Hubbard operators as the building-blocks of the Kronecker algebra of square matrices. Properties just as the composition of permutations are nicely worked in Hubbard notation. Some other properties as the Kronecker powers of operators $A^{\otimes k}$ are explicitly developed for their possible application in quantum control of multipartite systems. In Section 4 the useful notation of the direct sum of vector spaces and the linear representation of groups are also revisited while the Clebsch-Gordan problem is stated in general form. The second part of the paper is devoted to the applications. We first review the construction of irreducible representations of the $SU(2)$ Lie group in Hubbard notation (Section 5), then general expressions are derived for the representation of $SU(2) \times SU(2)$ in Hubbard notation (Section 6). In Section 7 the Clebsch-Gordan coefficients of the $SU(2) \times SU(2)$ Lie group are expressed in definite form by using the Hypergeometric function ${}_3F_2$. We close the paper with some concluding remarks. An

appendix is added to analyze some basic properties of the ceiling and floor functions that are required along the paper.

2 The Hubbard framework

Matrix calculus was developed for square matrices [29], and finds a lot of applications in quantum theory where the observables are represented by Hermitian operators. The latter are expressed as square matrices according to the representation defined by the measurable physical quantities and the related eigenvectors, see e.g. [30]. Any observable O of a quantum multipartite system $\mathcal{S} = \mathcal{S}_1 + \mathcal{S}_2 + \dots$ is defined on the entire Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots$, and can be expressed as matrix Kronecker products of the observables O_k belonging to the subsystems \mathcal{S}_k [13, 14]. We shall focus on the properties of square matrices in the understanding that they give a suitable linear representation of the group of observables defining a quantum system. Yet, most of the results we are going to derive can be immediately extended to the case of $n \times m$ matrices. However, some specific properties of square matrices require caution to be promoted to (or they simply can not be applied in) the rectangular case.

2.1 Notation and basic properties

Let the ket $|x\rangle$ be an element of the vector space \mathbb{K}^n , with \mathbb{K} a field which could be either \mathbb{R} or \mathbb{C} . This will be represented as a single-column matrix containing n numbers $x_i \in \mathbb{K}$. The latter will be indexed from 1 unless otherwise stated. Thus,

$$|x\rangle \in \mathbb{K}^n \quad \Rightarrow \quad |x\rangle = (x_1, x_2, \dots, x_n)^T, \quad x_k \in \mathbb{K}. \quad (9)$$

The size n of any n -tuple $|x\rangle$ will be implied whenever $|x\rangle$ be written as a linear combination of the orthonormal basis $\{|e_k^n\rangle\}_{k=1}^n$ of \mathbb{K}^n , otherwise this will be explicitly stated if necessary. Here $|e_k^n\rangle$ means the n -tuple which has a unity in the k -th position and all other entries equal to zero. The Hermitian transpose $|x\rangle^\dagger$ of any ket $|x\rangle \in \mathbb{K}^n$ will be represented by the bra $\langle x|$, this last is also called the dual of $|x\rangle$, defined as

$$|x\rangle^\dagger := \langle x| = (x_1^\dagger, x_2^\dagger, \dots, x_n^\dagger), \quad (10)$$

with $x_k^\dagger = x_k$ if $\mathbb{K} = \mathbb{R}$, and $x_k^\dagger = \bar{x}_k$ for $\mathbb{K} = \mathbb{C}$. The symbol \bar{z} stands for the complex conjugate of $z \in \mathbb{C}$. Note that the basis vectors are real, i.e. $|e_k^n\rangle^\dagger = |e_k^n\rangle^T = \langle e_k^n|$ is the n -dimensional row vector having 1 in the k -th position and 0 in all other entries. Therefore, the inner product between arbitrary basis elements is non-negative

$$\langle e_k^n | e_j^n \rangle = \delta_{kj}, \quad k, j \in \{1, 2, \dots, n\}. \quad (11)$$

So that any ket $|x\rangle \in \mathbb{K}^n$ can be also expressed as the linear combination

$$|x\rangle = \sum_{k=1}^n x_k |e_k^n\rangle, \quad x_\ell = \langle e_\ell^n | x \rangle \in \mathbb{K}. \quad (12)$$

In similar form,

$$\langle x| = \sum_{k=1}^n x_k^\dagger \langle e_k^n|, \quad x_\ell^\dagger = \langle x|e_\ell^n\rangle \in \mathbb{K}. \quad (13)$$

Hence, the inner product between $|x\rangle$ and $|y\rangle$, both arbitrary vectors in \mathbb{K}^n , is given by

$$\langle x|y\rangle = \sum_{k,\ell=1}^n x_k^\dagger y_\ell \langle e_k^n|e_\ell^n\rangle = \sum_{k=1}^n x_k^\dagger y_k. \quad (14)$$

Since $(\langle x|y\rangle)^\dagger = \langle y|x\rangle$, the space \mathbb{K}^n is Euclidean (Hermitian) with linear (sesquilinear) metric if $\mathbb{K} = \mathbb{R}$ ($\mathbb{K} = \mathbb{C}$) [15]. In general we shall write $\mathbb{K}^n = \text{Sp}\{|e_i^n\rangle\}_{i=1}^n$ to denote that \mathbb{K}^n is spanned by the orthonormal set $\{|e_1^n\rangle, |e_2^n\rangle, \dots, |e_n^n\rangle\}$, with $n \in \mathbb{N}$. In turn, $\text{Sp}\{|e_k^n\rangle\}$ will denote the one-dimensional space spanned by the single basis ket $|e_k^n\rangle$. From the inner product (14) one can identify every $\langle x|$ with a given mapping of \mathbb{K}^n into \mathbb{K} . The set of all these mappings is spanned by the duals of the basis vectors $|e_k^n\rangle$ and is included in the set of all the functionals $\mathbb{K}^n \rightarrow \mathbb{K}$. We write $\mathcal{K}^n = \text{Sp}\{\langle e_i^n|\}_{i=1}^n$ for such a dual vector space.

Now, using (12) and (10), the outer product between $|x\rangle$ and $|y\rangle$ yields the dyad

$$|x\rangle\langle y| = \sum_{i,j=1}^n x_i y_j^\dagger |e_i^n\rangle\langle e_j^n| \equiv \sum_{i,j=1}^n x_i y_j^\dagger X_n^{i,j}, \quad (15)$$

where the “dyadic” operators

$$X_n^{i,j} = |e_i^n\rangle\langle e_j^n|, \quad i, j = 1, 2, \dots, n \quad (16)$$

are represented by the matrices (8). The action of $|x\rangle\langle y|$ on \mathbb{K}^n produces the transition from the ket $|y\rangle$ to $|x\rangle$. In this sense, the matrix array

$$|x\rangle\langle y| = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} (y_1^\dagger, y_2^\dagger, \dots, y_n^\dagger) = \begin{pmatrix} x_1 y_1^\dagger & x_1 y_2^\dagger & \cdots & x_1 y_n^\dagger \\ x_2 y_1^\dagger & x_2 y_2^\dagger & \cdots & x_2 y_n^\dagger \\ \vdots & \vdots & \ddots & \vdots \\ x_n y_1^\dagger & x_n y_2^\dagger & \cdots & x_n y_n^\dagger \end{pmatrix} \quad (17)$$

is the linear representation of the transition operator $|x\rangle\langle y|$ in the vector space \mathbb{K}^n . In turn, the action of $X_n^{i,j}$ on the basis vector $|e_k^n\rangle$ gives

$$X_n^{i,j} |e_k^n\rangle = \delta_{jk} |e_i^n\rangle, \quad (18)$$

so that its action on any ket $|x\rangle$ in \mathbb{K}^n reads

$$X_n^{i,j} |x\rangle = x_j |e_i^n\rangle, \quad (19)$$

and its matrix elements are easily calculated

$$\langle e_i^n | X_n^{k,\ell} | e_j^n \rangle = \delta_{\ell j} \langle e_i^n | e_k^n \rangle = \delta_{\ell j} \delta_{ik}. \quad (20)$$

It is then clear that $X_n^{i,j}$ projects \mathbb{K}^n into the one-dimensional space $\text{Sp}\{|e_i^n\rangle\}$. The algebra of these operators is defined by the inner product, which can be set to coincide with the conventional matrix product, but it is simpler to use the algebraic rule

$$X_n^{i,j} X_n^{k,\ell} = |e_i^n\rangle\langle e_j^n|e_k^n\rangle\langle e_\ell^n| = \delta_{jk} X_n^{i,\ell}. \quad (21)$$

From (21), the following result is immediate

$$[X_n^{i,j}, X_n^{k,m}]_{\pm} = X_n^{i,j} X_n^{k,m} \pm X_n^{k,m} X_n^{i,j} = \delta_{jk} X_n^{i,m} \pm \delta_{mi} X_n^{k,j}. \quad (22)$$

On the other hand, the operators $X_n^{i,j}$ are noninvertible real matrices (i.e., $\det X_n^{i,j} = 0$, and $\overline{X_n^{i,j}} = X_n^{i,j}$) such that their transpose and adjoint (conjugate transpose) versions coincide

$$(X_n^{i,j})^\dagger = (X_n^{i,j})^T = X_n^{j,i}. \quad (23)$$

This last expression is easily verified by using (16) as follows

$$(X_n^{i,j})^T = (|e_i^n\rangle\langle e_j^n|)^T = (\langle e_j^n|)^T (|e_i^n\rangle)^T = |e_j^n\rangle\langle e_i^n| = X_n^{j,i}.$$

Note that the symmetric operators $X_n^{i,i}$ are Hermitian and satisfy the completeness relation

$$\mathbb{I}_n = \sum_{i=1}^n X_n^{i,i}. \quad (24)$$

Then, the matrices $X_n^{i,j}$ correspond to the linear representation of the Hubbard operators in the space \mathbb{K}^n , as all the properties (5) are verified.

The introduction of Hubbard operators in the algebra of operators representing quantum dynamical variables is very advantageous since substantial simplifications are achieved with the properties (21)–(24). Concrete realizations will be presented in the next sections, with special emphasis in the square matrix representation. Before that, some words concerning the case of rectangular matrices are necessary.

2.2 Rectangular matrices

To generalize the results of the previous section one would consider rectangular matrices. In contrast with the square matrices, a rectangular matrix transforms a vector in the space \mathcal{H}_n into a vector in the space \mathcal{H}_m where, in general, $\mathcal{H}_n \neq \mathcal{H}_m$. It is also well known that the multiplication of two rectangular matrices is defined only if the amount of columns of the first factor is equal to the number of rows of the second factor. Concerning the equivalent of the Hubbard operators in the rectangular case, let $E_{n \times m}^{i,j}$ be the $n \times m$ -elementary matrix having entry 1 in position (i, j) and all other entries equal to zero [5]. This can be expressed as

$$E_{n \times m}^{i,j} = |e_i^n\rangle\langle e_j^m|. \quad (25)$$

Note that $(E_{n \times m}^{i,j})^\dagger = (E_{n \times m}^{i,j})^T = E_{m \times n}^{j,i}$, so $(E_{n \times m}^{i,j})^\dagger$ and $E_{n \times m}^{i,j}$ are defined to act on different vector spaces for $n \neq m$, no matter the values of i and j . In the same context, the product between $n \times m$ -elementary matrices is constrained to the multiplication rule

$$E_{n \times m}^{i,j} E_{m \times p}^{k,\ell} = \delta_{jk} E_{n \times p}^{i,\ell}. \quad (26)$$

Thus, expressions like $E_{m \times p}^{k,\ell} E_{n \times m}^{i,j}$ are meaningless since the number of columns of $E_{m \times p}^{k,\ell}$ differs from the number of rows of $E_{n \times m}^{i,j}$. In spite of these apparent complications, the theorems of matrix calculus deduced for square matrices may be modified for the rectangular case. This is particularly right for the “square matrices in the broader sense” defined in [11], Ch. 2 (see also general expressions in [5]). As we have indicated, our interest is addressed to n -square matrices since they represent the most general linear operators in the vector space \mathbb{K}^n . The outline above is to stress that care must be taken with regard to the generalizations of our results to the rectangular case.

2.3 Square and permutation matrices

Using (16) it is easy to see that any n -square matrix $A = [a_{i,j}]$ can be expressed in terms of the Hubbard operators

$$A = \sum_{i,j=1}^n a_{i,j} X_n^{i,j}, \quad a_{i,j} \in \mathbb{K}, \quad (27)$$

so that the conventional matrix product AB is expressed as follows

$$AB = \left(\sum_{i,j=1}^n a_{i,j} X_n^{i,j} \right) \left(\sum_{k,\ell=1}^n b_{k,\ell} X_n^{k,\ell} \right) = \sum_{i,\ell=1}^n \left(\sum_k a_{i,k} b_{k,\ell} \right) X_n^{i,\ell} = C, \quad (28)$$

where C is the n -square matrix

$$C = \sum_{i,\ell=1}^n c_{i,\ell} X_n^{i,\ell}, \quad c_{i,\ell} = \sum_{k=1}^n a_{i,k} b_{k,\ell}. \quad (29)$$

The complex conjugate \overline{A} , the transpose A^T , and the adjoint A^\dagger of a matrix A read as

$$\overline{A} = \sum_{i,j=1}^n \overline{a}_{i,j} X_n^{i,j}, \quad A^T = \sum_{i,j=1}^n a_{i,j} X_n^{j,i}, \quad A^\dagger = \sum_{i,j=1}^n a_{i,j}^\dagger X_n^{j,i}. \quad (30)$$

On the other hand, the action of A on the basis vectors $|e_j^n\rangle$ is derived from (27) and (18), this gives

$$A|e_j^n\rangle = \sum_{k=1}^n a_{k,j} |e_k^n\rangle. \quad (31)$$

Then, for an arbitrary vector $|x\rangle$ in \mathbb{K}^n we have

$$A|x\rangle = \sum_{k,j,\ell=1}^n a_{k,j} x_\ell X_n^{k,j} |e_\ell^n\rangle = \sum_{k,\ell=1}^n a_{k,\ell} x_\ell |e_k^n\rangle. \quad (32)$$

The expression for the trace of a matrix is easily recovered:

$$\langle e_i^n | A | e_j^n \rangle = \sum_{k,\ell=1}^n a_{k,\ell} \delta_{i,k} \delta_{\ell,j} = a_{i,j} \quad \Rightarrow \quad \text{Tr} A = \sum_{i=1}^n \langle e_i^n | A | e_i^n \rangle = \sum_{i=1}^n a_{i,i}. \quad (33)$$

To give an example, consider a square matrix $H = [h_{i,j}]$ of size n consisting of unimodular entries, $|h_{i,j}| = 1$, and fulfilling $HH^\dagger = n\mathbb{I}_n$. This is called a Hadamard matrix³. In the simplest case, with $n = 2$ and real entries, we have

$$H = \frac{1}{\sqrt{2}} \sum_{i,j=1}^2 (-1)^{(i-1)(j-1)} X_2^{i,j} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad (34)$$

where the factor $1/\sqrt{2}$ has been introduced to make H unitary. Using (32) the action of H on $|x\rangle \in \mathbb{K}^2$ reads as

$$H|x\rangle = \frac{1}{\sqrt{2}} \sum_{i,k=1}^2 (-1)^{(i-1)(k-1)} x_k |e_i^2\rangle = \frac{1}{\sqrt{2}} [(x_1 + x_2)|e_1^2\rangle + (x_1 - x_2)|e_2^2\rangle]. \quad (35)$$

From (28), the multiplication of H with itself gives

$$H^2 = HH = \sum_{i,\ell=1}^2 c_{i,\ell} X_2^{i,\ell} = \mathbb{I}_2, \quad c_{i,\ell} = \frac{1 + (-1)^{i+\ell}}{2} = \delta_{i,\ell}. \quad (36)$$

As another example of interest consider a permutation defined by the bijection π of the set of natural numbers $S = \{1, \dots, n\}$ onto itself. In the Cauchy's two-line notation this map reads as

$$\pi = \begin{pmatrix} 1 & 2 & \dots & n \\ \pi(1) & \pi(2) & \dots & \pi(n) \end{pmatrix}.$$

In particular, the identical permutation π_e is such that $\pi_e(k) = k$ for all k in S . The set of all $n!$ permutations of S forms the symmetric (or permutation) group S_n of order n with the identity π_e as the unit element and the composition of maps as the product. Such a group plays an important role in quantum physics (see e.g. Ch. 13 of Ref. [11] and Ref. [15]). For example, the Schrödinger equation is invariant under the permutation of electrons since the physical equivalence of all these particles. A linear representation of S_n is obtained by assigning a matrix P_π per each permutation π . This is a square matrix of order n that has only one entry 1 per row and column, and is zero elsewhere. In Hubbard notation the matrix P_π reads in simple form

$$P_\pi = \sum_{j=1}^n X_n^{j,\pi(j)}. \quad (37)$$

³More precisely, the square matrices with ± 1 entries and having pairwise orthogonal rows are named after Hadamard [31]. These are included in the set of self-reciprocal matrices introduced by Sylvester [32]. Then, the definition above corresponds to a generalization of what is commonly known as a Hadamard matrix [19, 33].

In this representation the properties of permutation matrices can be studied in compact form. To give a pair of examples consider first the product of P_σ and P_π , two permutation matrices of order n . From (21) we have

$$P_\sigma P_\pi = \sum_{k,\ell=1}^n X_n^{k,\sigma(k)} X_n^{\ell,\pi(\ell)} = \sum_{k,\ell=1}^n \delta_{\sigma(k),\ell} X_n^{k,\pi(\ell)} = \sum_{k=1}^n X_n^{k,\pi(\sigma(k))} = P_{\pi \circ \sigma}. \quad (38)$$

Thus, the composition $\pi \circ \sigma$ of permutations π and σ is obtained from the product of the corresponding matrices. It is clear that the product of permutation matrices is non-commutative as $P_\pi P_\sigma = P_{\sigma \circ \pi}$ and $\sigma \circ \pi \neq \pi \circ \sigma$ in general. As a second example let us verify the orthogonality of permutation matrices $P_\pi^{-1} = P_{\pi^{-1}} = P_\pi^T$. From (30) and (21) one arrives at

$$P_\pi P_\pi^T = \sum_{k,\ell=1}^n \delta_{\pi(k),\pi(\ell)} X_n^{k,\ell} = \sum_{k=1}^n X_n^{k,k} = \mathbb{I}_n. \quad (39)$$

Similarly, $P_\pi^T P_\pi = \mathbb{I}_n$. From these results it follows the rule $(P_\sigma P_\pi)^{-1} = P_\pi^{-1} P_\sigma^{-1}$.

To close this section we emphasize that the action of P_π on any ket $|x\rangle \in \mathbb{K}^n$ is immediately calculated in Hubbard representation

$$P_\pi |x\rangle = \sum_{j,k=1}^n x_k X_n^{j,\pi(j)} |e_k^n\rangle = \sum_{j,k=1}^n x_k \delta_{\pi(j),k} |e_j^n\rangle = \sum_{j=1}^n x_{\pi(j)} |e_j^n\rangle. \quad (40)$$

In the next sections some of the properties of the Kronecker product of permutation matrices are going to be discussed.

3 Kronecker algebra in Hubbard representation

We start the analysis of the Kronecker algebra with the definition of the direct product.

Definition K1. Let $A = [a_{i,j}]$ and $B = [b_{r,s}]$ be respectively matrices of order $m \times n$ and $k \times \ell$ over the field \mathbb{K} . The Kronecker product $A \otimes B$ is the matrix of order $mk \times n\ell$ over the field \mathbb{K} defined as $A \otimes B = [a_{i,j} B]$.

As a first example consider the basis vectors $|e_k^n\rangle$, these are matrices of order $1 \times n$ so that $|e_k^n\rangle \otimes |e_j^n\rangle$ is a matrix of order $1 \cdot 1 \times n \cdot n = 1 \times n^2$. Moreover, this n^2 -tuple has only one unity at $(k-1)n + j$, and is zero in all other entries. In general, the Kronecker product of two basis vectors belonging to different spaces $|e_{i_1}^{n_1}\rangle$ and $|e_{i_2}^{n_2}\rangle$ gives a tuple of size $n_1 n_2$ that has a single unit among $n_1 n_2 - 1$ zeros, as this is stated in the following definition.

Definition K2. Let $|e_{i_1}^{n_1}\rangle$ and $|e_{i_2}^{n_2}\rangle$ be basis vectors of \mathbb{K}^{n_1} and \mathbb{K}^{n_2} respectively. Then the Kronecker product $|e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle$ is the $n_1 n_2$ -tuple having 1 at $(i_1-1)n_2 + i_2$, and zero in all other entries.

It is immediate to verify that the vectors constructed according to Definition K2 are orthonormal and that there are only $n_1 n_2$ of them. Thus, all of them represent an orthonormal basis of the vector space $\mathbb{K}^{n_1 n_2}$. We have the next proposition without giving a proof.

Proposition K0. Let $\mathbb{K}^{n_1} = \text{Sp} \{ |e_{i_1}^{n_1}\rangle \}_{i_1=1}^{n_1}$ and $\mathbb{K}^{n_2} = \text{Sp} \{ |e_{i_2}^{n_2}\rangle \}_{i_2=1}^{n_2}$ be vector spaces. The set of all the Kronecker products $|e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle$ is orthonormal and spans a vector space of dimension $n_1 n_2$, written $\mathbb{K}^{n_1 n_2} = \text{Sp} \{ |e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle, i_1 = 1, \dots, n_1; i_2 = 1, \dots, n_2 \}$, with the following axioms ($\alpha, \beta, \gamma, \eta$ are elements of \mathbb{K}):

- (i) $(\alpha |e_{i_1}^{n_1}\rangle) \otimes |e_{i_2}^{n_2}\rangle = \alpha(|e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle) = |e_{i_1}^{n_1}\rangle \otimes (\alpha |e_{i_2}^{n_2}\rangle)$
- (ii) $(\alpha |e_{i_1}^{n_1}\rangle + \beta |e_{i_1}^{n_1}\rangle) \otimes |e_{i_2}^{n_2}\rangle = \alpha(|e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle) + \beta(|e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle)$
- (iii) $|e_{i_1}^{n_1}\rangle \otimes (\gamma |e_{i_2}^{n_2}\rangle + \eta |e_{i_2}^{n_2}\rangle) = \gamma(|e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle) + \eta(|e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle)$

An arbitrary vector $|x\rangle \in \mathbb{K}^{n_1 n_2}$ can be written either as a twice-indexed linear combination

$$|x\rangle = \sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} x_{i_1, i_2} |e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle,$$

or as a single-indexed linear combination

$$|x\rangle = \sum_{k=1}^{n_1 n_2} \tilde{x}_k |e_k^{n_1 n_2}\rangle, \quad k = (i_1 - 1)n_2 + i_2.$$

Whenever this produces no confusion we shall write $|e_k^{n_1 n_2 n_3 \dots}\rangle$, $k = 1, 2, \dots, n_1 n_2 n_3 \dots$, to represent the basis vectors $|e_{i_1}^{n_1}\rangle \otimes |e_{i_2}^{n_2}\rangle \otimes |e_{i_3}^{n_3}\rangle \otimes \dots$, $i_\ell \in \{1, \dots, n_\ell\}$, that span $\mathbb{K}^{n_1 n_2 n_3 \dots}$. In particular, if $n_\ell = n$ for all $\ell \in \{1, \dots, p\}$, then

$$\mathbb{K}^{n^p} = \text{Sp} \left\{ |e_{i_1}^n\rangle \otimes \dots \otimes |e_{i_p}^n\rangle \right\}_{i_\ell=1}^n \quad (41)$$

is the space of contravariant tensors of rank p while its dual \mathcal{K}^{n^p} is the space of covariant tensors of rank p [15]. For instance, in quantum computing it is customary to write $|0\rangle$ and $|1\rangle$ for the basis vectors of \mathbb{K}^2 ; using our notation they are $|e_1^2\rangle$ and $|e_2^2\rangle$ respectively. According to Proposition K0, the four products $|e_{i_1}^2\rangle \otimes |e_{i_2}^2\rangle$, $i_\ell \in \{1, 2\}$, span \mathbb{K}^4 . These can be expressed in binary form as follows

$$\begin{aligned} |e_1^4\rangle &= |e_1^2\rangle \otimes |e_1^2\rangle = |0\rangle \otimes |0\rangle = |00\rangle, & |e_2^4\rangle &= |e_1^2\rangle \otimes |e_2^2\rangle = |0\rangle \otimes |1\rangle = |01\rangle, \\ |e_3^4\rangle &= |e_2^2\rangle \otimes |e_1^2\rangle = |1\rangle \otimes |0\rangle = |10\rangle, & |e_4^4\rangle &= |e_2^2\rangle \otimes |e_2^2\rangle = |1\rangle \otimes |1\rangle = |11\rangle. \end{aligned}$$

The same notation holds for an arbitrary number of two-dimensional factors. For instance,

$$|e_1^{32}\rangle = \underbrace{|e_1^2\rangle \otimes \dots \otimes |e_1^2\rangle}_{5 \text{ times}} = |00000\rangle.$$

3.1 Kronecker algebra of Hubbard operators

The Kronecker product $A \otimes B$ is simple if the factors are Hubbard operators (8). In this case, the resulting matrix has only one entry different from zero since each of the factors has a unique non zero entry. That is, the Kronecker product is closed in the set of Hubbard operators.

Proposition K1. Let $X_m^{i,j}$ and $X_n^{k,\ell}$ be two Hubbard operators of order n and m respectively. The Kronecker product $X_m^{i,j} \otimes X_n^{k,\ell}$ is the mn -Hubbard operator $X_{mn}^{n(i-1)+k, n(j-1)+\ell}$. That is,

$$X_m^{i,j} \otimes X_n^{k,\ell} = X_{mn}^{n(i-1)+k, n(j-1)+\ell}. \quad (42)$$

Proof. The proof follows from Definition K1, explicitly

$$\begin{aligned} & X_m^{i,j} \otimes X_n^{k,\ell} \\ &= \begin{pmatrix} & & & 0 & & & \\ & & & \vdots & & & \\ & 0_{(i-1) \times (j-1)} & & 0 & 0_{(i-1) \times (n-j)} & & \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ & & & 0 & & & \\ & & & \vdots & & & \\ & 0_{(n-i) \times (j-1)} & & 0 & 0_{(n-i) \times (n-j)} & & \end{pmatrix} \otimes X_n^{k,\ell} \\ &= \begin{pmatrix} & & & 0 & & & \\ & & & \vdots & & & \\ & 0_{[n(i-1)+k-1] \times [n(j-1)+\ell-1]} & & 0 & 0_{[n(i-1)+k-1] \times [mn-n(j-1)-\ell]} & & \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ & & & 0 & & & \\ & & & \vdots & & & \\ & 0_{[mn-n(i-1)-k] \times [n(j-1)+\ell-1]} & & 0 & 0_{[mn-n(i-1)-k] \times [n(j-1)+\ell-1]} & & \end{pmatrix} \\ &= X_{mn}^{n(i-1)+k, n(j-1)+\ell}. \quad \square \end{aligned}$$

Besides the basic property introduced in Proposition K1, the Kronecker algebra of the Hubbard operators includes the following set of properties.

Proposition K2. Let $X_\alpha^{\beta,\gamma}$ be Hubbard operators of order α and take $\lambda \in \mathbb{K}$. Then

- i) $X_m^{i,j} \otimes X_n^{k,\ell} \neq X_n^{k,\ell} \otimes X_m^{i,j}$ in general.
- ii) $(X_m^{i,j} \otimes X_n^{k,\ell})^T = (X_m^{i,j})^T \otimes (X_n^{k,\ell})^T$.
- iii) $(\lambda X_m^{i,j}) \otimes X_n^{k,\ell} = \lambda (X_m^{i,j} \otimes X_n^{k,\ell}) = X_m^{i,j} \otimes (\lambda X_n^{k,\ell})$.

- iv) $(X_m^{i,j} + X_m^{r,s}) \otimes X_n^{k,\ell} = X_m^{i,j} \otimes X_n^{k,\ell} + X_m^{r,s} \otimes X_n^{k,\ell}.$
- v) $X_n^{k,\ell} \otimes (X_m^{i,j} + X_m^{r,s}) = X_n^{k,\ell} \otimes X_m^{i,j} + X_n^{k,\ell} \otimes X_m^{r,s}$
- vi) $(X_m^{i,j} \otimes X_n^{k,\ell}) \otimes X_p^{r,s} = X_m^{i,j} \otimes (X_n^{k,\ell} \otimes X_p^{r,s}).$

Proof. Parts iii, iv and v are immediate from Definition K1.

i) From Proposition K1 we see that $X_m^{i,j} \otimes X_n^{k,\ell} = X_n^{k,\ell} \otimes X_m^{i,j}$ requires the roots of the system

$$n(i-1) + k = m(k-1) + i, \quad n(j-1) + \ell = m(\ell-1) + j,$$

which in general has no solution for arbitrary fixed values of n and m . A particular solution is obtained if $n = m$, for which one gets $i = k$ and $j = \ell$. The symmetric case $X_m^{i,j} \otimes X_m^{i,j}$ is recovered from this last result.

ii) From (42) and (23),

$$\begin{aligned} (X_m^{i,j} \otimes X_n^{k,\ell})^T &= \left(X_{mn}^{n(i-1)+k, n(j-1)+\ell} \right)^T = X_{mn}^{n(j-1)+\ell, n(i-1)+k} \\ &= X_m^{j,i} \otimes X_n^{\ell,k} = (X_m^{i,j})^T \otimes (X_n^{k,\ell})^T. \end{aligned}$$

Remark that this result immediately gives $(X_m^{i,j} \otimes X_n^{k,\ell})^\dagger = (X_m^{i,j})^\dagger \otimes (X_n^{k,\ell})^\dagger$, since the Hubbard operators are real matrices.

vi) From (42),

$$\begin{aligned} &(X_m^{i,j} \otimes X_n^{k,\ell}) \otimes X_p^{r,s} \\ &= X_{mn}^{n(i-1)+k, n(j-1)+\ell} \otimes X_p^{r,s} \\ &= X_{mnp}^{p[n(i-1)+k-1]+r, p[n(j-1)+\ell-1]+s} = X_{mnp}^{pn(i-1)+p(k-1)+r, pn(j-1)+p(\ell-1)+s} \\ &= X_m^{i,j} \otimes X_{np}^{p(k-1)+r, p(\ell-1)+s} = X_m^{i,j} \otimes (X_n^{k,\ell} \otimes X_p^{r,s}). \quad \square \end{aligned}$$

Proposition K2 includes the basic properties of the Kronecker product of Hubbard operators. Applied to the set $\{X_\alpha^{\beta,\gamma}\}$, they mean that the product \otimes is distributive over ordinary matrix addition (iv, v), associative (vi), compatible with ordinary matrix transposition (ii) as well as with matrix multiplication by an scalar (iii) and, in general, non-abelian (i). Next we generalize such properties to the case of arbitrary square matrices while some other algebraic relationships are derived.

3.2 Kronecker algebra of permutation matrices

The Kronecker algebra of the Hubbard operators is particularly useful in the operating with, and the construction of permutation matrices. In this section we report some results on permutation matrices that are fundamental in the ensuing applications of the Kronecker product. From Proposition K1 one has the following result.

Theorem P1. The square matrix

$$\Pi = \sum_{i,j=1}^n X_n^{i,j} \otimes X_n^{j,i} \quad (43)$$

is a permutation matrix of order n^2 , defined by the rule

$$\pi(p) = n(p + n - 1) - (n^2 - 1)p', \quad p = 1, 2, \dots, n^2, \quad (44)$$

with

$$p' = \left\lceil \frac{p}{n} \right\rceil \quad (45)$$

the ceiling function applied on $\frac{p}{n}$ (see Eq. (A.2) of the appendix).

Proof. From (42) we have

$$\Pi = \sum_{i,j=1}^n X_{n^2}^{n(i-1)+j, n(j-1)+i}.$$

Let us define $p = n(i - 1) + j$, then $p = 1, 2, \dots, ni$, and $j = p - n(i - 1)$. Therefore,

$$\Pi = \sum_{i=1}^n \sum_{p=n(i-1)+1}^{ni} X_{n^2}^{p, n(p+n-1)-(n^2-1)i},$$

with

$$\frac{p}{n} \leq i \leq \frac{p}{n} + 1 - \frac{1}{n} < \frac{p}{n} + 1. \quad (46)$$

Using Lemma A1(i) of the appendix we get

$$i = \left\lceil \frac{p}{n} \right\rceil \equiv p',$$

to write

$$\Pi = \sum_{p=1}^{n^2} X_{n^2}^{p, n(p+n-1)-(n^2-1)p'}.$$

Comparing this last result with (37) we arrive at the rule (44). It can be verified that $\pi(p)$ is indeed a bijection on the set $\{1, \dots, n^2\}$. \square

To get some insight on the meaning of the permutation matrix (43) let us consider an arbitrary contravariant tensor of rank 2:

$$|x_1\rangle \otimes |x_2\rangle = \sum_{i_1, i_2=1}^n x_{i_1} x_{i_2} |e_{i_1}^n\rangle \otimes |e_{i_2}^n\rangle = \sum_{i_1, i_2=1}^n x_{i_1} x_{i_2} |e_{(i_1-1)n+i_2}^{n^2}\rangle. \quad (47)$$

The action of Π on this last vector gives

$$\begin{aligned}\Pi(|x_1\rangle \otimes |x_2\rangle) &= \left(\sum_{i,j=1}^n X_n^{i,j} \otimes X_n^{j,i} \right) \left(\sum_{i_1,i_2=1}^n x_{i_1} x_{i_2} |e_{i_1}^n\rangle \otimes |e_{i_2}^n\rangle \right) \\ &= \sum_{i,j,i_1,i_2=1}^n x_{i_1} x_{i_2} \delta_{ji_1} \delta_{ii_2} |e_i^n\rangle \otimes |e_j^n\rangle = \sum_{i_1,i_2=1}^n x_{i_1} x_{i_2} |e_{i_2}^n\rangle \otimes |e_{i_1}^n\rangle \\ &= |x_2\rangle \otimes |x_1\rangle.\end{aligned}$$

Thus, relative to the indices labeling the contravariant tensor (47), the operator Π corresponds to the bijection $\pi_2 : (1, 2) \mapsto (2, 1)$. Hence $\Pi \equiv P_{\pi_2} \in S_2$. Indeed, there are only $2! = 2$ different permutations on the set $\{1, 2\}$, these are the identity $\pi_e \equiv \pi_1$ and π_2 . In Hubbard representation we have

$$P_{\pi_1} = \sum_{i,j=1}^n X_n^{i,i} \otimes X_n^{i,i} \equiv \sum_{i,j=1}^n \delta_{ij} X_n^{i,j} \otimes X_n^{j,i}, \quad P_{\pi_2} = \Pi. \quad (48)$$

From these results it is easy to verify that

$$\mathcal{S}_{(2)} = \frac{1}{2}(P_{\pi_1} + P_{\pi_2}) = \frac{1}{2} \sum_{i,j=1}^n (1 + \delta_{ij}) X_n^{i,j} \otimes X_n^{j,i} \quad (49)$$

is the symmetrization operator for the vectors in \mathbb{K}^{n^2} . Namely,

$$\mathcal{S}_{(2)}(|x_1\rangle \otimes |x_2\rangle) = \frac{|x_1\rangle \otimes |x_2\rangle + |x_2\rangle \otimes |x_1\rangle}{2}$$

is a symmetric tensor of rank 2. In a similar form, the operator

$$\mathcal{A}_{(2)} = \frac{1}{2} [\chi(\pi_1) P_{\pi_1} + \chi(\pi_2) P_{\pi_2}] = \frac{1}{2} \sum_{i,j=1}^n [\chi(\pi_1) + \chi(\pi_2) \delta_{ij}] X_n^{i,j} \otimes X_n^{j,i}, \quad (50)$$

with $\chi(\pi)$ the parity of the bijection π [15], produces antisymmetric tensors of rank 2:

$$\mathcal{A}_{(2)}(|x_1\rangle \otimes |x_2\rangle) = \frac{|x_1\rangle \otimes |x_2\rangle - |x_2\rangle \otimes |x_1\rangle}{2}.$$

The generalization of the above results to tensors of arbitrary rank is straightforward. We summarize this in the following proposition without a proof.

Proposition P1. The operators

$$\mathcal{S}_{(p)} = \frac{1}{p!} \sum_{\ell=1}^p P_{\pi_\ell} \quad \text{and} \quad \mathcal{A}_{(p)} = \frac{1}{p!} \sum_{\ell=1}^p \chi(\pi_\ell) P_{\pi_\ell} \quad (51)$$

with $\pi_\ell \in S_p$, $\pi_1 \equiv \pi_e$, and P_{π_ℓ} a definite linear combination of the Kronecker products

$$X_n^{i_1,j_1} \otimes X_n^{i_2,j_2} \otimes \dots \otimes X_n^{i_p,j_p}, \quad i_k, j_k \in \{1, \dots, n\},$$

produce respectively the symmetrization and antisymmetrization of the contravariant tensors of rank p .

The operators $\mathcal{S}_{(p)}$ and $\mathcal{A}_{(p)}$ are useful in group theory and symmetries [10, 11, 15, 17]. In the literature of combinatorics they appear in connection with the concepts of determinant and permanent of a matrix, these last give rise to entire treatises [34] and are associated to the concept of majorization of vectors that is fundamental in the algorithms of quantum computing [14] and in the geometry properties of the quantum states [35] as well. The symmetrization of vectors as this has been indicated above is also useful in the analysis of the Majorana representation of multi-qubit states for the studies of the barycentric measure of quantum entanglement [36]. The major result in Proposition P1 is that the Kronecker products defined in Theorem P1 as permutation matrices are nothing but the building blocks of the symmetrization and antisymmetrization operators of the contravariant vector space (41). The result reported in Theorem P1 has been already included in the works by other authors (see e.g. Eq. (4) of Ref. [1], and Section 2.5 of Ref. [5]) but, as far as we know, such works give no reference to the explicit form of the permutation. Here, equation (44) gives the concrete realization of such a permutation and the connection of Π with the operators (50) has been also achieved.

On the other hand, the Kronecker product of permutation matrices is also compatible with the composition of permutations described by equation (38). That is, the product \otimes is closed in the set of permutation matrices.

Theorem P2. Let $P_\pi(n)$ and $P_\sigma(m)$ be the n and m -permutation matrices defined by the rules π and σ respectively. The Kronecker product $P_\pi(n) \otimes P_\sigma(m)$ is the nm -permutation matrix $P_\alpha(n, m)$ defined by the rule

$$\alpha(p) = m[\pi(p') - 1] + \sigma(p - mp' + m), \quad (52)$$

with $p' = \lceil \frac{p}{m} \rceil$.

Proof. From Proposition K1 and the linearity of \otimes one gets

$$P_\alpha(n, m) = P_\pi(n) \otimes P_\sigma(m) = \sum_{i=1}^n \sum_{j=1}^m X_{nm}^{m(i-1)+j, m[\pi(i)-1]+\sigma(j)}.$$

Following the proof of Theorem P1 we realize that the change $p = m(i - 1) + j$ gives rise to equation (46) with $n \leftrightarrow m$, so that $p' = \lceil \frac{p}{m} \rceil$ and the rule (52) follows from the expression

$$P_\alpha(n, m) = \sum_{p=1}^{nm} X_{nm}^{p, m[\pi(p')-1]+\sigma(p-mp'+m)}.$$

Now, using the multiplication rule (21) and property (30) we have

$$P_\alpha^T(n, m) P_\alpha(n, m) = \sum_{p,q=1}^{nm} X_{nm}^{\alpha(p),p} X_{nm}^{q,\alpha(q)} = \sum_{p=1}^{nm} X_{nm}^{\alpha(p),\alpha(p)} = \mathbb{I}_{nm},$$

and a similar procedure shows that $P_\alpha(n, m) P_\alpha^T(n, m) = \mathbb{I}_{nm}$. \square

Now, let us consider Proposition K2(i). This indicates that the Kronecker product of two Hubbard operators, $X_n^{i,j}$ and $X_m^{k,\ell}$, is non-abelian in general. Such restriction, however, can be relaxed because $X_n^{i,j} \otimes X_m^{k,\ell}$ has only one entry 1, as this is established in Proposition K1; the same is true for $X_m^{k,\ell} \otimes X_n^{i,j}$. Therefore, it should be possible to arrive at $X_m^{k,\ell} \otimes X_n^{i,j}$ by applying the appropriate permutation of rows and columns in $X_n^{i,j} \otimes X_m^{k,\ell}$. That is, $X_n^{i,j} \otimes X_m^{k,\ell}$ and $X_m^{k,\ell} \otimes X_n^{i,j}$ must be permutation equivalent.

Proposition P2. The Kronecker product $X_n^{i,j} \otimes X_m^{k,\ell}$ is permutation equivalent to $X_m^{k,\ell} \otimes X_n^{i,j}$. That is, there exist P_π , a permutation matrix of order nm , such that

$$P_\pi^T (X_n^{i,j} \otimes X_m^{k,\ell}) P_\pi = X_m^{k,\ell} \otimes X_n^{i,j}. \quad (53)$$

Proof. We use the multiplication rule (21) and the expression (42), together with the linearity of \otimes , to arrive at

$$P_\pi^T (X_n^{i,j} \otimes X_m^{k,\ell}) P_\pi = X_{nm}^{\pi(mi-m+k), \pi(mj-m+\ell)}.$$

Hence, in order to satisfy (53) we have

$$\pi(mi - m + k) = nk - n + i. \quad (54)$$

The bijection π we are looking for is defined by this last equation (the labels j and ℓ satisfy the same equation under the change $i \rightarrow j$ and $k \rightarrow \ell$). \square

The permutation equivalence of matrix Kronecker products is of enormous interest in quantum information theory as this is useful in solving the problem of constructing maximally entangled bases of multipartite quantum systems. If dealing with Fourier matrices, it is possible to discriminate whether the permutation equivalence is preserved for the Kronecker products if matrix multiplication by unitary diagonal matrices is also allowed [19]. As discussed in the introduction, this problem deals with equation (3) for which the permutation matrices P_1 and P_2 are to be determined. The results we have presented in this section are addressed to show the basic operation rules of the permutation matrices when they are expressed as linear combinations of Hubbard operators. Further insights will be given in the sequel.

3.3 Kronecker algebra of square matrices

We now consider the properties of n -square matrices associated with the Kronecker product. One way to phrase the main subject of this section is to say that every n -square matrix A is a linear combination of Hubbard operators, just as this is stated in Eq. (27). In such a representation the assertions of the following propositions, theorems and corollaries are readily verified.

Theorem M1. The Kronecker product of $A = [a_{i,j}]$ and $B = [b_{k,\ell}]$, respectively n and m -square matrices, can be written as

$$A \otimes B = \sum_{i,j=1}^{nm} c_{i,j} X_{nm}^{i,j} \equiv C.$$

That is, the Kronecker product $A \otimes B$ is a linear combination of the Hubbard operators of order nm .

Proof. From Proposition K1 and the linearity of \otimes we have

$$A \otimes B = \sum_{i,j=1}^n \sum_{k,\ell=1}^m a_{i,j} b_{k,\ell} X_{mn}^{m(i-1)+k, m(j-1)+\ell}.$$

Let us define $p = m(i-1) + k$ and $q = m(j-1) + \ell$, so that $p, q = 1, \dots, mn$. Therefore $k = p - m(i-1)$ and $\ell = q - m(j-1)$. Hence,

$$A \otimes B = \sum_{i,j=1}^n \sum_{p=m(i-1)+1}^{ni} \sum_{q=m(j-1)+1}^{mj} a_{i,j} b_{p+m-mi, q+m-mj} X_{mn}^{p,q}.$$

The indexes i, p and m in the third sum are related by Eq. (46). The same is true for the indexes j, q and m in the fourth sum, so that according with Lemma A1(i) of the appendix we get

$$i = \left\lceil \frac{p}{m} \right\rceil := p', \quad j = \left\lceil \frac{q}{m} \right\rceil := q'. \quad (55)$$

Then

$$A \otimes B = \sum_{p,q=1}^{nm} c_{p,q} X_{mn}^{p,q}, \quad c_{p,q} := a_{p',q'} b_{p+m-mp', q+m-mq'}. \quad \square \quad (56)$$

As a first consequence of this theorem we realize that $A = \mathbb{I}_n$ and $B = \mathbb{I}_m$ produce $C = \mathbb{I}_{nm}$. That is, the Kronecker product of identity matrices is an identity matrix.

Corollary M1.1. The identity is preserved in the Kronecker product. That is $\mathbb{I}_n \otimes \mathbb{I}_m = \mathbb{I}_{nm}$

Proof. Use Theorem M1 with $a_{i,j} = \delta_{ij}$ and $b_{k,\ell} = \delta_{k\ell}$. \square

Another important consequence of Theorem M1 is that the nontrivial Kronecker powers of matrix A , written $A^{\otimes k+1}$ with $k \geq 1$, also admit a definite expression in Hubbard notation.

Corollary M1.2. The Kronecker product of the n -square matrix $A = [a_{i,j}]$ with itself $k \geq 1$ times, denoted $A^{\otimes k+1}$, is given by the expression

$$A^{\otimes k+1} = \sum_{p,q=1}^{n^{k+1}} a_{p,q}^{(k+1)} X_{n^{k+1}}^{p,q}, \quad k \geq 1, \quad (57)$$

with

$$a_{p,q}^{(k+1)} = a_{p_k,q_k} \prod_{s=0}^{k-1} a_{p_s+n-np_{s+1}, q_s+n-nq_{s+1}}, \quad (58)$$

and

$$p_s = \left\lfloor \frac{p}{n^s} \right\rfloor, \quad q_s = \left\lfloor \frac{q}{n^s} \right\rfloor, \quad s = 0, 1, \dots, k. \quad (59)$$

Proof. From Theorem M1, with $B = A$ in (56), one has

$$A^{\otimes 2} = \sum_{p,q=1}^{n^2} a_{p',q'} a_{p+n-np', q+n-nq'} X_{n^2}^{p,q},$$

with p' and q' as they have been introduced in (55). Applying again Theorem M1 with $A \leftrightarrow A^{\otimes 2}$ and $B \leftrightarrow A$ we get

$$A^{\otimes 2} \otimes A = \sum_{p,q=1}^{n^3} [a_{(p')',(q')'} a_{p'+n-n(p')', q'+n-n(q')'}] a_{p+n-np', q+n-nq'} X_{n^2}^{p,q} \quad (60)$$

where

$$(x')' = \left\lfloor \frac{x'}{n} \right\rfloor = \left\lfloor \frac{\left\lfloor \frac{x}{n} \right\rfloor}{n} \right\rfloor = \left\lfloor \frac{x}{n^2} \right\rfloor, \quad x = p, q.$$

In the last result we have used Lemma A1(iv) of the appendix. Here, it is convenient to use the notation introduced in (59), so that (60) reads as follows

$$\begin{aligned} A^{\otimes 3} &= \sum_{p,q=1}^{n^3} a_{p_2,q_2} a_{p_1+n-np_2, q_1+n-nq_2} a_{p_0+n-np_1, q_0+n-nq_1} X_{n^2}^{p,q} \\ &= \sum_{p,q=1}^{n^3} a_{p_2,q_2} \left(\prod_{s=0}^2 a_{p_s+n-np_{s+1}, q_s+n-nq_{s+1}} \right) X_{n^2}^{p,q} \\ &= \sum_{p,q=1}^{n^3} a_{p,q}^{(3)} X_{n^2}^{p,q}. \end{aligned}$$

The proof is completed by induction. \square

The action of $A^{\otimes t}$ on the vector space $\text{Sp} \{|e_\ell^n\rangle^{\otimes t}\}_{\ell=1}^n$ represents the parallel action of t operators A on t vector states $|\psi\rangle \in \text{Sp} \{|e_\ell^n\rangle\}_{\ell=1}^n$. This manifestation of the quantum parallelism is a fundamental feature of many quantum algorithms [14]. Thus, quantum circuits can be constructed to evaluate a function $f(x)$ for multiple values of x simultaneously. Most of the procedures implemented to calculate functions on an arbitrary number of bits use the Hadamard transform $H^{\otimes n}$. This operation is just n Hadamard operators acting in parallel on n qubits. It is then profitable to get a practical expression of $H^{\otimes n}$ as a particular application of Corollary M1.2.

Proposition M1.1. Let H be the Hadamard matrix (34), then

$$H^{\otimes k+1} = \frac{1}{\sqrt{2^{k+1}}} \sum_{p,q=1}^{2^{k+1}} (-1)^{\vec{p} \cdot \vec{q}} X_{2^{k+1}}^{p,q}, \quad k \geq 1, \quad (61)$$

with $p_s = \lceil \frac{p}{2^s} \rceil$, $q_s = \lceil \frac{q}{2^s} \rceil$, and

$$\vec{p} \cdot \vec{q} := \sum_{s=0}^k (p_s - 1)(q_s - 1). \quad (62)$$

Proof. For $n = 2$ and $A = H$, equations (57) and (58) respectively read as

$$H^{\otimes k+1} = \sum_{p,q=1}^{2^{k+1}} h_{p,q}^{(k+1)} X_{2^{k+1}}^{p,q}, \quad k \geq 1 \quad (63)$$

and

$$h_{p,q}^{(k+1)} = h_{p_k, q_k} \prod_{s=0}^{k-1} h_{p_s-2-2p_{s+1}, q_s-2-2q_{s+1}}, \quad x_s = \left\lceil \frac{x}{2^s} \right\rceil, \quad x = p, q.$$

From (34) we know that

$$h_{i,j} = 2^{-1/2} (-1)^{(i-1)(j-1)}, \quad i, j = 1, 2.$$

Therefore,

$$h_{p_s-2-2p_{s+1}, q_s-2-2q_{s+1}} = \frac{(-1)^{(p_s-2-2p_{s+1}-1)(q_s-2-2q_{s+1}-1)}}{\sqrt{2}} = \frac{(-1)^{(p_s-1)(q_s-1)}}{\sqrt{2}}$$

and

$$h_{p,q}^{(k+1)} = \frac{1}{\sqrt{2^{k+1}}} (-1)^{\sum_{s=0}^k (p_s-1)(q_s-1)}.$$

Equation (61) follows from the introduction of this last result in (63). \square

Let H_n denote a Hadamard matrix of order n ; the matrix H ($\equiv H_2$) defined in Eq. (34) and used in (61) is the simplest example. The next case is found for $n = 4$ as the orthogonality condition on the rows of H_n forces n to be even [33]. Proposition M1.1. gives an easy way to construct a Hadamard matrix of any order because $H^{\otimes k+1}$ is of size 2^{k+1} . For instance, $H_4 = H \otimes H = H^{\otimes 2}$ reads as follows

$$H_4 = H^{\otimes 2} = \frac{1}{2} \sum_{p,q=1}^4 (-1)^{(p-1)(q-1) + (\lceil \frac{p}{2} \rceil - 1)(\lceil \frac{q}{2} \rceil - 1)} X_4^{p,q} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}.$$

The matrices H_n are known as symmetric multiports (or Zeilinger matrices) in quantum optics [37] and have applications in combinatorial problems, coding algorithms and quantum engineering, among a diversity of subjects.

In order to appreciate the significance of Proposition M1.1., let us apply the operator $H^{\otimes k+1}$ on any of the vectors spanning $\mathbb{K}^{2^{k+1}}$. Using (61) and (31) with $A = H^{\otimes k+1}$ we get

$$H^{\otimes k+1}|e_j^{2^{k+1}}\rangle = \frac{1}{\sqrt{2^{k+1}}} \sum_{p=1}^{2^{k+1}} (-1)^{\sum_{s=0}^k (p_s-1)(j_s-1)} |e_p^{2^{k+1}}\rangle, \quad (64)$$

with $y_s = \lceil \frac{y}{2^s} \rceil$ for $y = p, j$. In particular, if $k = 1$ the latter expression gives

$$H^{\otimes 2}|e_j^4\rangle = \frac{1}{2} \sum_{p=1}^4 (-1)^{(p-1)(j-1)+(p_1-1)(j_1-1)} |e_p^4\rangle. \quad (65)$$

Explicitly,

$$2H^{\otimes 2}|e_j^4\rangle \rightarrow \begin{cases} |e_1^4\rangle + |e_2^4\rangle + |e_3^4\rangle + |e_4^4\rangle, & j = 1 \\ |e_1^4\rangle - |e_2^4\rangle + |e_3^4\rangle - |e_4^4\rangle, & j = 2 \\ |e_1^4\rangle + |e_2^4\rangle - |e_3^4\rangle - |e_4^4\rangle, & j = 3 \\ |e_1^4\rangle - |e_2^4\rangle - |e_3^4\rangle + |e_4^4\rangle, & j = 4 \end{cases}$$

We can see that the action of $H^{\otimes 2}$ on $|e_1^4\rangle$ produces an equal superposition of all basis states. In quantum computing, this corresponds to set an empty quantum register of 2 qubits $|00\rangle \equiv |e_1^4\rangle$ into an equally weighted distribution of all the basis states of the register $|00\rangle$, $|01\rangle = |e_2^4\rangle$, $|10\rangle = |e_3^4\rangle$ and $|11\rangle = |e_4^4\rangle$. At this stage, it would be useful to show the translation of the results from our notation to the binary one, which is widely used in the quantum computing context. We first give the following definition.

Definition M1.1. Consider a positive integer $x \leq 2^{k+1}$ with $k \in \mathbb{N}$. The expansion of x in powers of 2 is defined by the binary coefficients $x_s \in \{0, 1\}$, $s = 0, 1, \dots, k+1$, as follows

$$x = \sum_{i=0}^{k+1} x_i 2^i. \quad (66)$$

Now we pay attention to the coefficients of the linear combination (61), as only these must be rewritten to get equations (61) and (64) in binary form. The next proposition is necessary.

Proposition M1.2. Let p and q be respectively the i -th and j -th powers of 2 with $i, j = 0, 1, \dots, k+1$, and $k \in \mathbb{N}$. Then

$$(-1)^{\sum_{s=0}^k (\lceil \frac{p}{2^s} \rceil - 1)(\lceil \frac{q}{2^s} \rceil - 1)} = (-1)^{\sum_{s=0}^k (p-1)_s (q-1)_s}, \quad (67)$$

where $(p-1)_s$ and $(q-1)_s$ are the s -th binary coefficients of $p-1$ and $q-1$ respectively.

Proof. We first prove the identity

$$(-1)^{\sum_{s=0}^k \lfloor \frac{p}{2^s} \rfloor \lfloor \frac{q}{2^s} \rfloor} = (-1)^{\sum_{s=0}^k p_s q_s}, \quad (68)$$

with $\lfloor x \rfloor$ the floor function of x (see Eq. (A.3) of the appendix). Using the binary expansion of p and q we can write

$$\left\lfloor \frac{p}{2^s} \right\rfloor \left\lfloor \frac{q}{2^s} \right\rfloor = \sum_{i,j=0}^{k+1} \lfloor p_i 2^{i-s} \rfloor \lfloor q_j 2^{j-s} \rfloor, \quad s = 0, 1, 2, \dots, k. \quad (69)$$

Given s one has $\lfloor x_\ell 2^{\ell-s} \rfloor = 0$ for $x_\ell \in \{0, 1\}$ and $\ell < s$, since $0 \leq x_\ell 2^{\ell-s} < 1$. Then, all the terms labelled with either $i < s$ or $j < s$ in (69) are equal to zero. We have four partial sums

$$\left\lfloor \frac{p}{2^s} \right\rfloor \left\lfloor \frac{q}{2^s} \right\rfloor = \lfloor p_s \rfloor \lfloor q_s \rfloor + \lfloor p_s \rfloor \sum_{j=s+1}^{k+1} \lfloor q_j 2^{j-s} \rfloor + \lfloor q_s \rfloor \sum_{i=s+1}^{k+1} \lfloor p_i 2^{i-s} \rfloor + \sum_{i,j=s+1}^{k+1} \lfloor p_i 2^{i-s} \rfloor \lfloor q_j 2^{j-s} \rfloor.$$

The second and third terms of this last result are either zero or an even number, so they can be omitted from the exponent of -1 in the expression at the left of Eq. (68). The same can be said of the fourth term after the change $i - s \rightarrow r$, $j - s \rightarrow t$. Finally, $\lfloor p_s \rfloor \lfloor q_s \rfloor = p_s q_s$ since $p_s, q_s \in \{0, 1\}$. Therefore, taking into account only the elements of (69) that contribute in nontrivial form to the exponent of -1 we get (68). That is,

$$\left\lfloor \frac{p}{2^s} \right\rfloor \left\lfloor \frac{q}{2^s} \right\rfloor \stackrel{*}{=} p_s q_s \quad \Rightarrow \quad (-1)^{\sum_{s=0}^k \lfloor \frac{p}{2^s} \rfloor \lfloor \frac{q}{2^s} \rfloor} = (-1)^{\sum_{s=0}^k p_s q_s}.$$

Using Lemma A1 (part v) of the appendix and this last result, equation (67) follows. \square

To verify the compatibility of our results with those obtained in a binary representation let us rewrite the coefficients of the linear combination (64) according to Proposition M1.2. For $k = 1$ one has

$$H^{\otimes 2} |e_j^4\rangle = \frac{1}{2} \sum_p^4 (-1)^{(p-1)_0(j-1)_0 + (p-1)_1(j-1)_1} |e_p^4\rangle, \quad (70)$$

which explicitly gives the following result

$$2H^{\otimes 2} |e_j^4\rangle \rightarrow \begin{cases} (-1)^{0\cdot 0+0\cdot 0} |e_1^4\rangle + (-1)^{1\cdot 0+0\cdot 0} |e_2^4\rangle + (-1)^{0\cdot 0+0\cdot 1} |e_3^4\rangle + (-1)^{1\cdot 0+1\cdot 0} |e_4^4\rangle, & j = 1 \\ (-1)^{0\cdot 1+0\cdot 0} |e_1^4\rangle + (-1)^{1\cdot 1+0\cdot 0} |e_2^4\rangle + (-1)^{0\cdot 1+1\cdot 0} |e_3^4\rangle + (-1)^{1\cdot 1+1\cdot 0} |e_4^4\rangle, & j = 2 \\ (-1)^{0\cdot 0+0\cdot 1} |e_1^4\rangle + (-1)^{1\cdot 0+0\cdot 1} |e_2^4\rangle + (-1)^{0\cdot 0+1\cdot 1} |e_3^4\rangle + (-1)^{0\cdot 1+1\cdot 1} |e_4^4\rangle, & j = 3 \\ (-1)^{0\cdot 1+0\cdot 1} |e_1^4\rangle + (-1)^{1\cdot 1+0\cdot 1} |e_2^4\rangle + (-1)^{0\cdot 1+1\cdot 1} |e_3^4\rangle + (-1)^{1\cdot 1+1\cdot 1} |e_4^4\rangle, & j = 4 \end{cases}$$

The comparison of (70) with (64) shows that the results are consistent in both representations. The final step is to express $|e_j^4\rangle$ in binary form. Using Proposition K0 and Definition M1.1 we make

$$|e_j^{2^{k+1}}\rangle \rightarrow |j-1\rangle_{(k)} := |(j-1)_0, (j-1)_1, \dots, (j-1)_k\rangle,$$

with $(j-1)_s \in \{0, 1\}$ the binary coefficients of $j-1$ up to 2^k . If $k=1$ then $|e_j^4\rangle \rightarrow |j-1\rangle_{(1)} = |(j-1)_0, (j-1)_1\rangle$. Hence $|e_1^4\rangle \rightarrow |0\rangle_{(1)} = |0, 0\rangle$, so that we can write $|e_1^4\rangle = |00\rangle$, and so on. Then, we can write equation (64) in the standard form

$$H^{\otimes n}|x\rangle = \frac{1}{\sqrt{2^n}} \sum_z (-1)^{x \cdot z} |z\rangle,$$

where $n = 2^{k+1}$. Here $|x\rangle$ and $|z\rangle$ are in binary notation.

Coming back to Theorem M1, we stress that this can be generalized to an arbitrary number of factors by including the products $A \otimes B$ and $A^{\otimes k+1}$ as particular cases. This is stated in the following proposition.

Proposition M1.3. Let $A_r = [a_{i,j}^{(r)}]$ be a square matrix of order n_r . The Kronecker product $A_1 \otimes A_2 \otimes \dots \otimes A_{k+1}$ is the square matrix of order $n^{(k)} = n_1 n_2 \dots n_{k+1}$, expressed as the following linear combination of Hubbard operators

$$A = A_1 \otimes A_2 \otimes \dots \otimes A_{k+1} = \sum_{p,q=1}^{n^{(k)}} \tilde{a}_{p,q}^{(k)} X_{n^{(k)}}^{p,q}, \quad k \geq 1, \quad (71)$$

where

$$\tilde{a}_{p,q}^{(k)} = a_{p_k, q_k}^{(1)} \prod_{s=0}^{k-1} a_{p_s + n_{k-s+1} - n_{k-s+1} p_{s+1}, q_s + n_{k-s+1} - n_{k-s+1} q_{s+1}}^{(k-s+1)}, \quad (72)$$

and

$$p_s = \left\lceil \frac{p}{\prod_{\ell=1}^s n_{k-\ell+2}} \right\rceil, \quad q_s = \left\lceil \frac{q}{\prod_{\ell=1}^s n_{k-\ell+2}} \right\rceil. \quad (73)$$

Proof. This is immediate by following the proof of Theorem M1 and Corollary M1.2. \square

The advantage of having an expression for the matrix Kronecker product as general as the one reported in Proposition M1.3 relies on the fact that this includes an arbitrary number of factors, the size of which is in turn arbitrary. Immediate results can be obtained as particular cases. For instance, if $k=1$ and $a_{i,j}^{(1)} = a_{i,j}$, $a_{i,j}^{(2)} = b_{i,j}$, the product (71) gives the expression of $A \otimes B$ reported in Theorem M1. Now, let all factors in (71) be of the same order, namely $n_r = n$ for $r = 1, 2, \dots, k+1$, then the coefficient (72) reads as

$$\tilde{a}_{p,q}^{(k)} = a_{p_k, q_k}^{(1)} \prod_{s=0}^{k-1} a_{p_s + n - n p_{s+1}, q_s + n - n q_{s+1}}^{(k-s+1)}, \quad (74)$$

and the definitions of p_s and q_s in (73) are reduced to the ones given in (59). Using these last results and considering the situation in which all the factors are equal, i.e. $A_r = A$ for all r , one recovers the expression for $A^{\otimes k+1}$ reported in Corollary M1.2. In such a case, the super-index could be omitted from all the matrix elements appearing in (74). On the other hand, let A_r be Fourier matrices F_r , then (71) is the ‘Fourier Kronecker product’ defined in [38], expanded in terms of Hubbard operators. In addition, this is ‘factored’ if the size n_r of the matrices A_r are natural powers of prime numbers, and is called ‘pure factored’ if such powers are ordered:

$$F = F_{a^{\ell_1}} \otimes F_{a^{\ell_2}} \otimes \cdots \otimes F_{a^{\ell_{k+1}}}, \quad \ell_1 \gg \ell_2 \gg \cdots \gg \ell_{k+1}, \quad \ell_j \in \mathbb{N},$$

where a is a prime number. The immediate generalization considers $n_r = a_r^{\ell_r}$, with a_r standing for a prime number and $r = 1, \dots, k+1$. In Ref. [38], a ‘multi-index’ notation is also introduced to operate the above mentioned products. Such notation works well for the necessities indicated by its author in the study of Fourier matrices. However, it could be not easy to generalize this to the Kronecker algebra of square matrices other than the Fourier ones. In contradistinction, the algebraic rules presented here are based on the linear superposition of Hubbard operators, so that they minimize the number of indices that are required to operate with. In this form, the Hubbard representation facilitates the calculation of the Kronecker algebra of the square matrices of any sort.

Theorem M2. Let $A = [a_{i,j}]$, $C = [c_{p,q}]$, and $B = [b_{k,\ell}]$, $D = [d_{r,s}]$, be pairs of n and m -square matrices respectively. The usual matrix product of the nm -square matrices $A \otimes B$ and $C \otimes D$ fulfills

$$(A \otimes B)(C \otimes D) = AC \otimes BD. \quad (75)$$

That is, the Kronecker product of square matrices is compatible with ordinary matrix multiplication.

Proof. From Proposition K1 and the linearity of \otimes one arrives at

$$\begin{aligned} A \otimes B &= \sum_{i,j}^n \sum_{k,\ell}^m a_{i,j} b_{k,\ell} X_{mn}^{m(i-1)+k, m(j-1)+\ell}, \\ C \otimes D &= \sum_{p,q}^n \sum_{r,s}^m c_{p,q} d_{r,s} X_{mn}^{m(p-1)+r, m(q-1)+s}. \end{aligned}$$

Using (21) and Lemma A2 of the appendix we get

$$\begin{aligned}
(A \otimes B)(C \otimes D) &= \sum_{i,j,p,q}^n \sum_{k,\ell,r,s}^m a_{i,j} b_{k,\ell} c_{p,q} d_{r,s} \delta_{m(p-1)+r, m(j-1)+\ell} X_{mn}^{m(i-1)+k, m(q-1)+s} \\
&= \sum_{i,j,q}^n \sum_{k,\ell,s}^m (a_{i,j} c_{j,q}) (b_{k,\ell} d_{\ell,s}) X_{mn}^{m(i-1)+k, m(q-1)+s} \\
&= \sum_{i,q}^n \sum_{k,s}^m (AC)_{i,q} (BC)_{k,s} X_{mn}^{m(i-1)+k, m(q-1)+s} \\
&= \left(\sum_{i,q}^n (AC)_{i,q} X_m^{i,q} \right) \otimes \left(\sum_{k,s}^m (BD)_{k,s} X_n^{k,s} \right) = AC \otimes BD. \quad \square
\end{aligned}$$

At this stage we have to stress that Theorem M2 can be extended to rectangular matrices whenever the involved matrix products make sense (see the discussion of Section 2.2). This fact will be taken into account in e.g., Corollary TM2.2 and Proposition G.1.

Corollary TM2.1. Let A and D be square matrices of order n and m respectively. Then the following relationship holds

$$A \otimes D = (A \otimes \mathbb{I}_m)(\mathbb{I}_n \otimes D). \quad (76)$$

Proof. Use $B = \mathbb{I}_m$ and $C = \mathbb{I}_n$ in Theorem M2. \square

Corollary TM2.2. Consider the eigenvalue equations $A|a_i\rangle = \alpha_i|a_i\rangle$ and $B|b_j\rangle = \beta_j|b_j\rangle$, with $i = 1, 2, \dots, n$ and $j = 1, 2, \dots, m$. Then (i) the nm numbers $\alpha_i\beta_j$ are the eigenvalues of $A \otimes B$ associated to the vectors $|a_i\rangle \otimes |b_j\rangle$ (ii) The eigenvalues of $A \otimes \mathbb{I}_m + \mathbb{I}_n \otimes B$ are the numbers $\alpha_i + \beta_j$.

Proof. Using (12) the vectors $|a_i\rangle$ and $|b_j\rangle$ can be represented by row tuples of size n and m respectively. Then, Theorem M2 applies as follows

$$(A \otimes B)(|a_i\rangle \otimes |b_j\rangle) = A|a_i\rangle \otimes B|b_j\rangle = \alpha_i\beta_j (|a_i\rangle \otimes |b_j\rangle),$$

and the proof of (i) is completed. In similar form,

$$(A \otimes \mathbb{I}_m + \mathbb{I}_n \otimes B)(|a_i\rangle \otimes |b_j\rangle) = A|a_i\rangle \otimes \mathbb{I}_m|b_j\rangle + \mathbb{I}_n|a_i\rangle \otimes B|b_j\rangle = (\alpha_i + \beta_j)(|a_i\rangle \otimes |b_j\rangle)$$

completes the proof of (ii). \square

The following properties are presented here in connection with the Kronecker algebra of Hubbard operators, because any square matrix can be expressed as a linear combination of such operators. In this form, the proof of each item is simple by using equation (27) and Proposition K2.

Theorem M3. Let A, B and C be n -square matrices and $\lambda \in \mathbb{K}$. Then

- i) In general, $A \otimes B \neq B \otimes A$.
- ii) $(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger$ and $(A \otimes B)^T = A^T \otimes B^T$.
- iii) $(\lambda A) \otimes B = \lambda(A \otimes B) = A \otimes (\lambda B)$.
- iv) $(A + B) \otimes C = A \otimes C + B \otimes C$.
- v) $A \otimes (B + C) = A \otimes B + A \otimes C$.
- vi) $(A \otimes B) \otimes C = A \otimes (B \otimes C)$.

Proof. The theorem follows from Proposition K2 and properties (27) and (30). For instance, the proof of both parts in (ii) is quite similar:

$$\begin{aligned}
(A \otimes B)^\dagger &= \left[\left(\sum_{i,j=1}^n a_{i,j} X_n^{i,j} \right) \otimes \left(\sum_{k,\ell=1}^n b_{k,\ell} X_n^{k,\ell} \right) \right]^\dagger = \left(\sum_{i,j,k,\ell=1}^n a_{i,j} b_{k,\ell} X_n^{i,j} \otimes X_n^{k,\ell} \right)^\dagger \\
&= \sum_{i,j,k,\ell=1}^n \overline{a_{i,j} b_{k,\ell}} (X_n^{i,j} \otimes X_n^{k,\ell})^\dagger = \sum_{i,j,k,\ell=1}^n \bar{a}_{i,j} \bar{b}_{k,\ell} (X_n^{i,j})^\dagger \otimes (X_n^{k,\ell})^\dagger \\
&= A^\dagger \otimes B^\dagger.
\end{aligned}$$

Then $(A \otimes B)^T = (\overline{A \otimes B})^\dagger = \overline{A}^\dagger \otimes \overline{B}^\dagger = A^T \otimes B^T$. \square

As for Proposition K2, the above properties mean that the Kronecker product is distributive over ordinary matrix addition (iv, v), associative (vi), compatible with ordinary matrix transposition (ii) and the matrix multiplication by an scalar (iii). Remarkably, although the product \otimes is non-abelian for arbitrary square matrices (i), it is possible to set equivalence classes between Kronecker products that are ‘abelian’ up to a permutation matrix. Our claim is based on the Proposition P2 as well as the linearity of the Hubbard operators and leads to the following theorem.

Theorem M4. Let $A = [a_{i,j}]$ and $B = [b_{k,\ell}]$ be two square matrices of order n and m respectively. The Kronecker product $A \otimes B$ is permutation equivalent to $B \otimes A$.

Proof. From Proposition P2 we know that there exists a permutation matrix P such that (53) is true. Then, by linearity in the conventional matrix product we have

$$\begin{aligned}
P^T(A \otimes B)P &= \sum_{i,j}^n \sum_{k,\ell}^m a_{i,j} b_{k,\ell} [P^T (X_n^{i,j} \otimes X_m^{k,\ell}) P] \\
&= \sum_{i,j}^n \sum_{k,\ell}^m b_{k,\ell} a_{i,j} X_m^{k,\ell} \otimes X_n^{i,j} = B \otimes A. \quad \square
\end{aligned}$$

The next properties show that the Kronecker product is compatible with the conventional measure properties of square matrices.

Proposition M1.4. Let $A = [a_{i,j}]$ and $B = [b_{k,\ell}]$ be two square matrices of order n and m respectively. Then

$$\text{Tr}(A \otimes B) = \text{Tr}(A)\text{Tr}(B) = \text{Tr}(B \otimes A).$$

Proof. Using Proposition K1, the linearity of \otimes , and property (20) we can write

$$\langle e_s^{nm} | A \otimes B | e_s^{nm} \rangle = \sum_{i,j}^n \sum_{k,\ell}^m a_{i,j} b_{k,\ell} \delta_{s, m(i-1)+k} \delta_{m(j-1)+\ell, s}.$$

Then, (33) gives

$$\begin{aligned} \text{Tr}(A \otimes B) &= \sum_s^{nm} \langle e_s^{nm} | A \otimes B | e_s^{nm} \rangle = \sum_{i,j}^n \sum_{k,\ell}^m a_{i,j} b_{k,\ell} \delta_{m(i-1)+k, m(j-1)+\ell} \\ &= \sum_{i,j}^n \sum_{k,\ell}^m a_{i,j} b_{k,\ell} \delta_{i,j} \delta_{k,\ell} = \left(\sum_i^n a_{i,i} \right) \left(\sum_k^m b_{k,k} \right) \\ &= \text{Tr}(A)\text{Tr}(B) = \text{Tr}(B)\text{Tr}(A) = \text{Tr}(B \otimes A), \end{aligned}$$

where we have used Lemma A2 of the appendix. \square

Proposition M1.5. Let $A = [a_{i,j}]$ and $B = [b_{k,\ell}]$ be two n -square matrices. Then

$$\text{Det}(A \otimes B) = (\text{Det } A)^n (\text{Det } B)^n. \quad (77)$$

Proof. From Corollary TM2.1 we have

$$A \otimes B = (A \otimes \mathbb{I}_n)(\mathbb{I}_n \otimes B).$$

Then

$$\text{Det}(A \otimes B) = \text{Det}(A \otimes \mathbb{I}_n) \text{Det}(\mathbb{I}_n \otimes B) = \text{Det}(A \otimes \mathbb{I}_n) (\text{Det } B)^n.$$

The last term in the previous expression is because $\mathbb{I}_n \otimes B$ is a Jordan matrix having n repetitions of B along the diagonal. Now we use Theorem M4 to get

$$\text{Det} [P^T (A \otimes \mathbb{I}_n) P] = \text{Det}(A \otimes \mathbb{I}_n) = \text{Det}(\mathbb{I}_n \otimes A) = (\text{Det } A)^n.$$

Equation (77) follows from the above results. \square

Additional properties (and proofs) of the Kronecker product of matrices can be found in the books [5–7]. The most recent summary of the properties of the \otimes operation has been reported in [9] (see also [8]). Although these references are addressed to the case of rectangular matrices, most of the useful applications of the product \otimes require square matrices only. Indeed, properties like the permutation equivalence of Kronecker products are fundamental in the simplification of algorithms to process data or in the study of symmetries associated to a given physical system, among other applications of square matrices. Next, we shall apply our results in the analysis of the angular momentum of quantum systems.

4 Basics of the Clebsch-Gordan decomposition

In this section we consider the Kronecker product of two irreducible representations of a given group. Our interest here is to analyze the generalities of the reduction of such a product as a sum of irreducible representations. To start with, we require some basic definitions of the direct sum of vector spaces and the linear representation of groups.

4.1 Direct sum of vector spaces

Definition S1. Let $\mathcal{H} = \mathcal{H}' \oplus \mathcal{H}''$ be the direct sum vector space of \mathcal{H}' and \mathcal{H}'' over the field \mathbb{K} . Then $\mathcal{H}' \cap \mathcal{H}'' = \text{Sp}\{|\emptyset\rangle\}$, with $|\emptyset\rangle$ the null vector of \mathcal{H} . Assuming $\text{Dim}(\mathcal{H}) < \infty$, we have $\text{Dim}(\mathcal{H}) = \text{Dim}(\mathcal{H}') + \text{Dim}(\mathcal{H}'')$. In general, any vector $|x\rangle \in \mathcal{H}$ can be written in the form of a two-vector tuple $|x\rangle = (|x'\rangle, |x''\rangle)^T$, with $|x'\rangle \in \mathcal{H}'$ and $|x''\rangle \in \mathcal{H}''$. The following matrix notation will often be used

$$|x\rangle = \begin{pmatrix} x_1 \\ \vdots \\ x_{n'} \\ x_{n'+1} \\ \vdots \\ x_{n'+n''} \end{pmatrix} \equiv |x'\rangle \oplus |x''\rangle = \begin{pmatrix} |x'\rangle \\ |x''\rangle \end{pmatrix} \equiv \begin{pmatrix} x'_1 \\ \vdots \\ x'_{n'} \\ x''_1 \\ \vdots \\ x''_{n''} \end{pmatrix}.$$

Now, let $A' : \mathcal{H}' \rightarrow \mathcal{H}'$ and $A'' : \mathcal{H}'' \rightarrow \mathcal{H}''$ be respectively automorphisms of \mathcal{H}' and \mathcal{H}'' . Assume their action is as follows

$$A'|x'\rangle = |y'\rangle, \quad A''|x''\rangle = |y''\rangle.$$

They together can be expressed in a single matrix operator acting on the entire space $\mathcal{H}' \oplus \mathcal{H}''$ in block-diagonal form

$$\left(\begin{array}{c|c} A' & 0_{n' \times n''} \\ \hline 0_{n'' \times n'} & A'' \end{array} \right) \begin{pmatrix} |x'\rangle \\ |x''\rangle \end{pmatrix} = \begin{pmatrix} |y'\rangle \\ |y''\rangle \end{pmatrix}.$$

We shall write in this case $A = A' \oplus A''$, and we shall say that the automorphism $A : \mathcal{H} \rightarrow \mathcal{H}$ decomposes into the direct sum of A' and A'' .

Definition S2. Let $\mathcal{H} = \mathcal{H}' \oplus \mathcal{H}''$ be the direct sum of vector spaces \mathcal{H}' and \mathcal{H}'' , with $\text{Dim}(\mathcal{H}') = n'$ and $\text{Dim}(\mathcal{H}'') = n''$. The direct sum operator $A = A' \oplus A''$, written in diagonal matrix form as

$$A = A' \oplus A'' = \left(\begin{array}{c|c} A' & 0_{n' \times n''} \\ \hline 0_{n'' \times n'} & A'' \end{array} \right),$$

is defined to act on $|x\rangle = |x'\rangle \oplus |x''\rangle \in \mathcal{H}$ as $A|x\rangle = (A' \oplus A'')|x\rangle = A'|x'\rangle \oplus A''|x''\rangle$, with $A' \in \text{Aut}(\mathcal{H}')$ and $A'' \in \text{Aut}(\mathcal{H}'')$ respectively.

Hereafter $\text{Aut}(X)$ denotes the set of all automorphisms of X . The next proposition allows to distinguish between operators that can be decomposed as a direct sum when they act on any vector space $\bigoplus_k \mathcal{H}_k$, and those that act on $\bigoplus_k \mathcal{H}_k$ in a more complicated manner.

Proposition S1. The most general operator acting on the direct sum space $\mathcal{H} = \mathcal{H}' \oplus \mathcal{H}''$ is of the form

$$A = \left(\begin{array}{c|c} A' & B \\ \hline C & A'' \end{array} \right),$$

with B and C matrices of order $n' \times n''$ and $n'' \times n'$ which respectively maps \mathcal{H}'' into \mathcal{H}' and \mathcal{H}' into \mathcal{H}'' . A' and A'' are n' and n'' -square matrices respectively.

Proof. The proof is immediate in matrix notation

$$A|x\rangle = \left(\begin{array}{cc} A' & B \\ C & A'' \end{array} \right) \left(\begin{array}{c} |x'\rangle \\ |x''\rangle \end{array} \right) = \left(\begin{array}{c} A'|x'\rangle + B|x''\rangle \\ C|x'\rangle + A''|x''\rangle \end{array} \right),$$

where the products $B|x''\rangle$ and $C|x'\rangle$ are $n' \times 1$ and $n'' \times 1$ matrices respectively. \square

4.2 Linear representation of groups

Definition G1. Let G and \mathcal{H} be a group and a vector space respectively. The homomorphism

$$\begin{aligned} T : G &\rightarrow \text{Aut}(\mathcal{H}) \\ g &\mapsto T(g) \end{aligned}$$

is a linear representation of G on \mathcal{H} . The vector space \mathcal{H} is called the representation space induced by T . The operator $T(g)$ fulfills

$$T(g_2 g_1) = T(g_2) T(g_1), \quad \forall g_1, g_2 \in G.$$

Henceforth all the operators will be expressed in matrix form, so that the representations considered will be linear.

Definition G2. Given a representation T of G on \mathcal{H} , a subspace \mathcal{H}_s of \mathcal{H} is said to be G -invariant if, for all $|x\rangle \in \mathcal{H}_s$ and all $g \in G$, we have $T(g)|x\rangle \in \mathcal{H}_s$, i.e., $T(g) \in \text{Aut}(\mathcal{H}_s)$ for all $g \in G$. In any representation there exist two trivial invariant subspaces; \mathcal{H} itself and the null vector space $\text{Sp}\{|\emptyset\rangle\}$. A representation T of G on \mathcal{H} is irreducible, written $\Delta(G)$, if the only G -invariant subspaces of \mathcal{H} are $\text{Sp}\{|\emptyset\rangle\}$ and \mathcal{H} itself.

Proposition G1. Let $\Delta'(G)$ and $\Delta''(G)$ be two irreducible representations of a given group G . Let $\text{Dim}(\mathcal{H}') = n'$ and $\text{Dim}(\mathcal{H}'') = n''$ be the dimensions of the corresponding representation spaces. Given $g \in G$, the Kronecker product of matrices $\Delta'(g)$ and $\Delta''(g)$ is a square matrix of order $n'n''$ acting on $\mathcal{H}' \otimes \mathcal{H}''$. That is, the set of matrices

$$(\Delta' \otimes \Delta'')(g) = \Delta'(g) \otimes \Delta''(g)$$

defines a linear representation of the product $G \times G$, with $\mathcal{H}' \otimes \mathcal{H}''$ as the representation space.

Proof. Given $|x'\rangle \in \mathcal{H}'$ and $|x''\rangle \in \mathcal{H}''$, one has $\Delta'(g)|x'\rangle = |y'\rangle \in \mathcal{H}'$ and $\Delta''(g)|x''\rangle = |y''\rangle \in \mathcal{H}''$. Using Theorem M2 we obtain

$$(\Delta'(g) \otimes \Delta''(g))(|x'\rangle \otimes |x''\rangle) = \Delta'(g)|x'\rangle \otimes \Delta''(g)|x''\rangle = |y'\rangle \otimes |y''\rangle = |y\rangle.$$

Therefore, given $g \in G$, there exists a matrix $T(g) = \Delta'(g) \otimes \Delta''(g) \in \text{Aut}(\mathcal{H}' \otimes \mathcal{H}'')$ such that $T(g)|x\rangle = |y\rangle$, with $|x\rangle = |x'\rangle \otimes |x''\rangle$ and $|y\rangle = |y'\rangle \otimes |y''\rangle$. \square

4.3 Clebsch-Gordan decomposition

Let us stress that in general the Kronecker product $\Delta' \otimes \Delta''$ is not irreducible, even though Δ' and Δ'' are irreducible. This unpleasant situation defines the problem of reducing $\Delta' \otimes \Delta''$ as much as possible to a representation where the vector space \mathcal{H} is G -invariant. The best we can do is to split the representation space \mathcal{H} into a set of subspaces $\mathcal{H}_k \cap \mathcal{H}_j = \text{Sp}\{|\emptyset\rangle\}$, $k \neq j$, each of them being G -invariant. Then, $\Delta' \otimes \Delta''$ is decomposed into a set of irreducible representations Δ_k , one per each subspace \mathcal{H}_k .

Definition G3. Let $\Delta'(G)$ and $\Delta''(G)$ be two irreducible representations of a given group G . The Clebsch-Gordan decomposition of $(\Delta' \otimes \Delta'')(g)$ is the reduction of the Kronecker product $\Delta'(g) \otimes \Delta''(g)$ into a direct sum of ρ irreducible representations $\Delta_k(g)$ defined as

$$(\Delta' \otimes \Delta'')(g) = \bigoplus_{k=1}^{\rho} \Delta_k(g) = \Delta_1(g) \oplus \Delta_2(g) \oplus \cdots \oplus \Delta_{\rho}(g), \quad \forall g \in G.$$

Note that the representation space of the Clebsch-Gordan decomposition $\bigoplus_{k=1}^{\rho} \Delta_k$ is the direct sum $\bigoplus_{k=1}^{\rho} \mathcal{H}_k$. Therefore, Definition G3 implies that the vector space $\mathcal{H}' \otimes \mathcal{H}''$ is decomposed into the direct sum $\mathcal{H}' \otimes \mathcal{H}'' = \bigoplus_{k=1}^{\rho} \mathcal{H}_k$. If it is possible to solve the Clebsch-Gordan decomposition problem for a given product $\Delta' \otimes \Delta''$ we say that such representation is *completely reducible*. Remark that only finite dimensional representations are always completely reducible, for infinite dimensional representations this is not generally true [11].

5 The group $SU(2)$ in Hubbard representation

Let us consider the group of unimodular (i.e., with determinant +1) unitary 2×2 matrices $SU(2)$. The general form of one of these matrices is

$$A = \begin{pmatrix} a & b \\ -\bar{b} & \bar{a} \end{pmatrix}, \quad |a|^2 + |b|^2 = 1. \quad (78)$$

In terms of the identity \mathbb{I}_2 and the Pauli matrices $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, with

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (79)$$

equation (78) reads

$$A = a_0 \mathbb{I}_2 + i\vec{a} \cdot \vec{\sigma}, \quad \vec{a} = (a_1, a_2, a_3), \quad a = a_0 + ia_3, \quad b = a_2 + ia_1.$$

The well known correspondence between the elements of $SU(2)$ and the points of a sphere of radius π in the three-dimensional euclidean space makes clear that this Lie group is not only compact and connected, but it is also simply connected [17]. The Lie algebra of $SU(2)$ is usually defined in terms of the Hermitian operators $T_k = \frac{1}{2}\sigma_k$, $k = 1, 2, 3$. That is, the basis of the representation $T(SU(2))$ satisfies the angular momentum algebra

$$[T_k, T_\ell] = i\epsilon_{k\ell m} T_m, \quad (80)$$

with $\epsilon_{k\ell m}$ the Levi-Civita symbol. The $SU(2)$ group is of rank 1 (there is not a pair of independent elements of the algebra (80) that commute among themselves), and the analysis of the structure constants $c_{k\ell}^m = i\epsilon_{k\ell m}$ shows that this is actually simple. Therefore, one can confine the study of $SU(2)$ to the construction of the corresponding finite-dimensional irreducible representations. Remark that the set $\{T_1, T_2, T_3\}$ is indeed an irreducible two-dimensional representation, as this is defined on the vector space $\text{Sp}\{|e_1^2\rangle, |e_2^2\rangle\}$. We are interested in the more general situation where the algebra (80) induces complex representation spaces \mathcal{H} with $\text{Dim}(\mathcal{H}) = n \geq 2$.

Let Δ be an n -dimensional irreducible representation of $T(SU(2))$ in \mathcal{H} , then the operators $\Delta(T_k)$ are complex n^2 -square matrices. We define

$$J_3 = \Delta(T_3), \quad J_\pm = [\Delta(T_1) \pm i\Delta(T_2)], \quad (81)$$

so that

$$[J_+, J_-] = 2J_3, \quad [J_3, J_\pm] = \pm J_\pm, \quad (82)$$

and

$$J_3^\dagger = J_3, \quad J_\pm^\dagger = J_\mp. \quad (83)$$

5.1 Irreducible representation of $SU(2)$

From (82) one realizes that J_\pm are raising and lowering operators for the eigenvectors of J_3 . Indeed, let $|\varphi\rangle$ be such that $J_3|\varphi\rangle = \alpha|\varphi\rangle$, then

$$J_3 J_\pm |\varphi\rangle = (\alpha \pm 1) J_\pm |\varphi\rangle \quad \Rightarrow \quad J_3 J_\pm^r |\varphi\rangle = (\alpha \pm r) J_\pm^r |\varphi\rangle, \quad r \in \mathbb{N}. \quad (84)$$

Remark that the non-vanishing vectors $J_\pm^r |\varphi\rangle$ are linearly independent as they belong to different eigenvalues of J_3 . Let $|\varphi_{ext}\rangle$ be such that $J_3|\varphi_{ext}\rangle = j|\varphi_{ext}\rangle$ and $J_+|\varphi_{ext}\rangle = 0$. The eigenvalue j corresponds to the highest weight of the representation since the extremal state $|\varphi_{ext}\rangle$ is annihilated by J_+ (otherwise the representation would be not finite dimensional). In the same context we should have $J_-^m |\varphi_{ext}\rangle = 0$ for some positive integer m . Let $s+1$ be the smallest value of m for which this is true, then one can verify that necessarily $s = 2j$. In this form, according to s , the highest weight j is either a half

integer or an integer. The representation Δ is therefore $2j + 1$ -dimensional and this is characterized by the highest weight j . For the related representation space we have

$$\mathcal{H} = \text{Sp}\{|\varphi_{ext}\rangle, J_-|\varphi_{ext}\rangle, \dots, J_-^{2j-1}|\varphi_{ext}\rangle, J_-^{2j}|\varphi_{ext}\rangle\}, \quad \text{Dim}(\mathcal{H}) = n = 2j + 1. \quad (85)$$

Now let $|\varphi_r\rangle := J_-^r|\varphi_{ext}\rangle$, $r = 0, 1, \dots, 2j$. Using (82) and (83) one gets

$$J_+|\varphi_r\rangle = (2J_3 + J_-J_+)J_-^{r-1}|\varphi_{ext}\rangle = 2(j+1-r)|\varphi_{r-1}\rangle + J_-J_+|\varphi_{r-1}\rangle.$$

After r iterations we obtain

$$J_+|\varphi_r\rangle = 2 \left[r(j+1-r) + \sum_{\ell=1}^{r-1} \ell \right] |\varphi_{r-1}\rangle,$$

so that

$$J_+|\varphi_r\rangle = r(2j+1-r)|\varphi_{r-1}\rangle. \quad (86)$$

Then, applying (83) and after $r-1$ iterations, from (86) we obtain the normalization constant

$$\langle\varphi_r|\varphi_r\rangle = \langle\varphi_{r-1}|J_+|\varphi_r\rangle = r(2j+1-r)\langle\varphi_{r-1}|\varphi_{r-1}\rangle = \frac{r!(2j)!}{(2j-r)!}\langle\varphi_{ext}|\varphi_{ext}\rangle = C_r^2. \quad (87)$$

Hereafter we shall assume $\langle\varphi_{ext}|\varphi_{ext}\rangle = 1$.

The normalized states $C_{r=j-m}^{-1}|\varphi_{r=j-m}\rangle$, $m = -j, \dots, j$, integrate an orthonormal set of eigenvectors belonging to J_3 . For these, it is customary to use the following notation

$$|j, m\rangle := \frac{1}{C_{j-m}}|\varphi_{j-m}\rangle = \sqrt{\frac{(j+m)!}{(2j)!(j-m)!}}|\varphi_{j-m}\rangle, \quad m = -j, \dots, j, \quad (88)$$

where the first entrance of $|j, m\rangle$ refers to the highest weight j and the second one to the eigenvalue m of J_3 that labels the specific member of the basis we are dealing with. The representation space (85) is then rewritten as

$$\mathcal{H} = \text{Sp}\{|j, j\rangle, |j, j-1\rangle, \dots, |j, -j+1\rangle, |j, -j\rangle\} = \text{Sp}\{|j, m\rangle\}_{m=j}^{-j}. \quad (89)$$

The basis operators (81) act on this last vector space as follows

$$\begin{aligned} J_3|j, m\rangle &= m|j, m\rangle, \\ J_+|j, m\rangle &= \sqrt{(j-m)(j+m+1)}|j, m+1\rangle, \\ J_-|j, m\rangle &= \sqrt{(j+m)(j-m+1)}|j, m-1\rangle. \end{aligned} \quad (90)$$

5.2 Hubbard operators

In order to express the set $\{J_3, J_\pm\}$ in Hubbard notation let us introduce the change

$$m \leftrightarrow m_k = j + 1 - k, \quad \text{with } k = 1, \dots, 2j + 1. \quad (91)$$

Then $|j, m\rangle \leftrightarrow |j, m_k\rangle \equiv |j, j + 1 - k\rangle$, and we can define

$$X_n^{p,q} := |j, m_p\rangle \langle j, m_q| \equiv |j, j + 1 - p\rangle \langle j, j + 1 - q|, \quad n = 2j + 1. \quad (92)$$

In this notation the diagonal matrix J_3 reads in simple form

$$J_3 = \sum_{k=1}^n m_k X_n^{k,k}, \quad n = 2j + 1. \quad (93)$$

Using the linearity of the Hubbard operators and property (18), it is straightforward to verify the first of equations (90):

$$J_3 |j, m\rangle = \sum_{k=1}^n m_k (X_n^{k,k} |j, m_s\rangle) = \sum_{k=1}^n m_k \delta_{k,s} |j, m_k\rangle = m_s |j, m_s\rangle = m |j, m\rangle,$$

where we have used (91). In a similar form we have the irreducible representation of the raising and lowering operators

$$J_+ = \sum_{k=1}^{n-1} \sqrt{k(2j+1-k)} X_n^{k,k+1}, \quad J_- = \sum_{k=1}^{n-1} \sqrt{k(2j+1-k)} X_n^{k+1,k}. \quad (94)$$

For completeness, let us express equations (90) in the “ k ”-representation defined in (91)-(92). We have

$$\begin{aligned} J_3 |j, m_k\rangle &= m_k |j, m_k\rangle, \\ J_+ |j, m_k\rangle &= \sqrt{(k-1)(2j+2-k)} |j, m_{k-1}\rangle, \\ J_- |j, m_k\rangle &= \sqrt{k(2j+1-k)} |j, m_{k+1}\rangle. \end{aligned} \quad (95)$$

Since the Hubbard operators $X_n^{i,j}$ are real matrices, using (23) in (93) and (94), it is now easy to verify the relationships (83). For simplicity, it is also convenient to introduce the notation

$$c_k^2 = k(2j+1-k). \quad (96)$$

Remark that

$$\prod_{i=1}^k c_i^2 = C_k^2,$$

with C_k^2 defined in (87). Hence, the expressions (94) can be rewritten as

$$J_+ = \sum_{k=1}^{n-1} c_k X_n^{k,k+1} \quad \text{and} \quad J_- = \sum_{k=1}^{n-1} c_k X_n^{k+1,k}. \quad (97)$$

The first three lowest dimensional irreducible representations of $SU(2)$ are reported below. In all cases there is agreement with the matrix representation obtained in conventional form reported in e.g. [40].

5.2.1 Highest weight $j = 1/2$.

The lowest dimension of the representation space \mathcal{H} is obtained for the weight $j = 1/2$. Thus $\mathcal{H}_{1/2} = \text{Sp}\{|\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle\}$, with $\text{Dim}(\mathcal{H}_{1/2}) = 2$ and

$$J_z^{(1/2)} = \frac{1}{2}X_2^{1,1} - \frac{1}{2}X_2^{2,2} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}, \quad (98)$$

$$J_+^{(1/2)} = X_2^{1,2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad J_-^{(1/2)} = X_2^{2,1} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

5.2.2 Highest weight $j = 1$.

For $j = 1$ we have $\mathcal{H}_1 = \text{Sp}\{|1, 1\rangle, |1, 0\rangle, |1, -1\rangle\}$ and $\text{Dim}(\mathcal{H}_1) = 3$, with

$$J_z^{(1)} = X_3^{1,1} - X_3^{3,3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad (99)$$

$$J_+^{(1)} = \sqrt{2}X_3^{1,2} + \sqrt{2}X_3^{2,3} = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} = \left(J_-^{(1)}\right)^\dagger.$$

5.2.3 Highest weight $j = 3/2$.

For $j = 3/2$ we have $\mathcal{H}_{3/2} = \text{Sp}\{|\frac{3}{2}, \frac{3}{2}\rangle, |\frac{3}{2}, \frac{1}{2}\rangle, |\frac{3}{2}, -\frac{1}{2}\rangle, |\frac{3}{2}, -\frac{3}{2}\rangle\}$, with $\text{Dim}(\mathcal{H}_{3/2}) = 4$ and

$$J_z^{(3/2)} = \frac{3}{2}X_4^{1,1} + \frac{1}{2}X_4^{2,2} - \frac{1}{2}X_4^{3,3} - \frac{3}{2}X_4^{4,4} = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}, \quad (100)$$

$$J_+^{(3/2)} = \sqrt{3}X_4^{1,2} + 2X_4^{2,3} + \sqrt{3}X_4^{3,4} = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} = \left(J_-^{(3/2)}\right)^\dagger.$$

6 $SU(2) \times SU(2)$ in Hubbard notation

In this section we solve the Clebsch-Gordan problem associated to the Kronecker product of two irreducible representations of $SU(2)$. That is, we are going to find the invariant subspaces that integrate the complete representation space of $SU(2) \times SU(2)$ as a direct sum.

6.1 The product of irreducible representations

Let Δ_1 and Δ_2 be two irreducible representations of $T(SU(2))$ with j_1 and j_2 the corresponding highest weights. Denote

$$\mathcal{H}_{j_s} = \text{Sp}\{|j_s, m^{(j_s)}\rangle \mid m^{(j_s)} = -j_s, \dots, j_s\}, \quad s = 1, 2,$$

the related representation spaces. Therefore

$$\mathcal{H}_{(j_1, j_2)} = \text{Sp}\{|j_1, m^{(j_1)}\rangle \otimes |j_2, m^{(j_2)}\rangle \mid m^{(j_s)} = -j_s, \dots, j_s, s = 1, 2\} \quad (101)$$

is the $n_1 n_2$ -dimensional representation space of $\Delta^{(j_1, j_2)} = \Delta_1 \otimes \mathbb{I}_{n_2} + \mathbb{I}_{n_1} \otimes \Delta_2$, with $n_1 = 2j_1 + 1$ and $n_2 = 2j_2 + 1$. Remark that $\Delta^{(j_1, j_2)}$ is not necessarily an irreducible representation. As the basis of operators we shall use in each space

$$J_3^{(j_s)} = \Delta_s(T_3), \quad J_{\pm}^{(j_s)} = [\Delta_s(T_1) \pm i\Delta_s(T_2)], \quad s = 1, 2. \quad (102)$$

Following (91-97), in Hubbard notation we write

$$J_3^{(j_s)} = \sum_{k=1}^{n_s} m_k^{(j_s)} X_{n_s}^{k,k}, \quad J_+^{(j_s)} = \sum_{k=1}^{n_s-1} c_k^{(j_s)} X_{n_s}^{k,k+1}, \quad J_-^{(j_s)} = \sum_{k=1}^{n_s-1} c_k^{(j_s)} X_{n_s}^{k+1,k}, \quad (103)$$

with

$$m_k^{(j_s)} = (j_s + 1 - k), \quad c_k^{(j_s)} = \sqrt{k(2j_s + 1 - k)}, \quad n_s = 2j_s + 1, \quad s = 1, 2. \quad (104)$$

We now promote the latter operators to act on the entire vector space (101). Thus, the operators

$$J_3^{(j_1, j_2)} = J_3^{(j_1)} \otimes \mathbb{I}_{n_2} + \mathbb{I}_{n_1} \otimes J_3^{(j_2)}, \quad J_{\pm}^{(j_1, j_2)} = J_{\pm}^{(j_1)} \otimes \mathbb{I}_{n_2} + \mathbb{I}_{n_1} \otimes J_{\pm}^{(j_2)} \quad (105)$$

correspond to the basis of $SU(2) \times SU(2)$ in the representation defined by the vector space $\mathcal{H}_{(j_1, j_2)}$. It is straightforward to verify the commutation rules

$$[J_+^{(j_1, j_2)}, J_-^{(j_1, j_2)}] = 2J_3^{(j_1, j_2)}, \quad [J_3^{(j_1, j_2)}, J_{\pm}^{(j_1, j_2)}] = \pm J_{\pm}^{(j_1, j_2)}, \quad (106)$$

and the relationships

$$\left(J_3^{(j_1, j_2)}\right)^{\dagger} = J_3^{(j_1, j_2)}, \quad \left(J_{\pm}^{(j_1, j_2)}\right)^{\dagger} = J_{\mp}^{(j_1, j_2)}. \quad (107)$$

In Hubbard notation the matrix representation of the operators (105) read as

$$J_3^{(j_1, j_2)} = \sum_{k=1}^{n_1} \sum_{\ell=1}^{n_2} \left(m_k^{(j_1)} + m_{\ell}^{(j_2)}\right) X_{n_1 n_2}^{n_2(k-1)+\ell, n_2(k-1)+\ell}, \quad (108)$$

and

$$J_+^{(j_1, j_2)} = \sum_{k=1}^{n_1-1} \sum_{\ell=1}^{n_2} c_k^{(j_1)} X_{n_1 n_2}^{n_2(k-1)+\ell, n_2 k+\ell} + \sum_{r=1}^{n_1} \sum_{t=1}^{n_2-1} c_t^{(j_2)} X_{n_1 n_2}^{n_2(r-1)+t, n_2(r-1)+t+1}. \quad (109)$$

Using Theorem M1 one can simplify the above expressions to get

$$J_3^{(j_1, j_2)} = \sum_{p=1}^{n_1 n_2} \left[m_{p'}^{(j_1)} + m_{p+n_2-n_2 p'}^{(j_2)} \right] X_{n_1 n_2}^{p, p} \quad (110)$$

and

$$J_+^{(j_1, j_2)} = \sum_{p=1}^{n_2(n_1-1)} c_{p'}^{(j_1)} X_{n_1 n_2}^{p, p+n_2} + \sum_{p=1}^{n_1 n_2-1} c_{p+n_2-n_2 p'}^{(j_2)} X_{n_1 n_2}^{p, p+1}, \quad (111)$$

where $p' = \lceil \frac{p}{n_2} \rceil$. As an example let us show the explicit form of some of the matrices (111). In all the following examples we use $c_1^{(\frac{1}{2})} = 1$ and $c_1^{(1)} = c_2^{(1)} = \sqrt{2}$. Our results can be compared with those obtained in conventional form reported in e.g. [40].

6.1.1 Weights $j_1 = \frac{1}{2}$ and $j_2 = \frac{1}{2}$

$$J_+^{(\frac{1}{2}, \frac{1}{2})} = c_1^{(\frac{1}{2})} (X_4^{1,3} + X_4^{2,4} + X_4^{1,2} + X_4^{3,4}) = \left(\begin{array}{cc|cc} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{array} \right). \quad (112)$$

6.1.2 Weights $j_1 = \frac{1}{2}$ and $j_2 = 1$

$$\begin{aligned} J_+^{(\frac{1}{2}, 1)} &= c_1^{(\frac{1}{2})} (X_6^{1,4} + X_6^{2,5} + X_6^{3,6}) + c_1^{(1)} (X_6^{1,2} + X_6^{4,5}) + c_2^{(1)} (X_6^{2,3} + X_6^{5,6}) \\ &= \left(\begin{array}{ccc|ccc} 0 & \sqrt{2} & 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right). \end{aligned} \quad (113)$$

6.1.3 Weights $j_1 = 1, j_2 = \frac{1}{2}$

$$\begin{aligned}
J_+^{(1, \frac{1}{2})} &= c_1^{(1)} (X_6^{1,3} + X_6^{2,4}) + c_2^{(1)} (X_6^{3,5} + X_6^{4,6}) + c_1^{(\frac{1}{2})} (X_6^{1,2} + X_6^{3,4}) \\
&= \left(\begin{array}{ccc|ccc} 0 & 1 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 1 & \sqrt{2} & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right). \tag{114}
\end{aligned}$$

6.2 Irreducible representation

We want to decompose the $n_1 n_2$ -dimensional space $\mathcal{H}_{(j_1, j_2)}$ into a direct sum of irreducible subspaces. Using the additivity of eigenvalues in the Kronecker product (see Corollary TM2.2), we realize that $j_1 + j_2$ is the highest weight of $J_3^{(j_1, j_2)}$. Given $j_1 + j_2 - k + 1$, there are k different pairs of weights $m^{(j_1)}$ and $m^{(j_2)}$ such that $m^{(j_1)} + m^{(j_2)} = j_1 + j_2 - k + 1$. For $k = 1$ there is only one way to get $m^{(j_1)} + m^{(j_2)} = j_1 + j_2$, therefore we have a single state $|j_1, j_1\rangle \otimes |j_2, j_2\rangle$ in $\mathcal{H}_{(j_1, j_2)}$ belonging to the highest weight $j = j_1 + j_2$. According to the discussion of Section 5.1, $|j_1, j_1\rangle \otimes |j_2, j_2\rangle$ is the extremal state of a vector space $\mathcal{H}_{j_1+j_2} \subset \mathcal{H}_{(j_1, j_2)}$ in which the matrix basis $\{T_1, T_2, T_3\}$ is irreducible. Denote $\Delta_{j_1+j_2}$ such an irreducible representation and write $\{J_3^{(j_1+j_2)}, J_{\pm}^{(j_1+j_2)}\}$ for the basis operators. Then

$$\mathcal{H}_{j_1+j_2} = \text{Sp}\{|j, j\rangle, J_-^{(j_1+j_2)}|j, j\rangle, J_-^{(j_1+j_2)+1}|j, j\rangle, \dots, J_-^{2(j_1+j_2)}|j, j\rangle\}$$

with $|j, j\rangle \equiv |j_1, j_1\rangle \otimes |j_2, j_2\rangle$. In this form, $\text{Dim}(\mathcal{H}_{j_1+j_2}) = 2(j_1 + j_2) + 1$ and the vector space (101) is rewritten as the direct sum $\mathcal{H}_{(j_1, j_2)} = \mathcal{H}_{j_1+j_2} \oplus \mathcal{H}_R$, with $\mathcal{H}_R \subset \mathcal{H}_{(j_1, j_2)}$ such that $\mathcal{H}_{j_1+j_2} \cap \mathcal{H}_R = \text{Sp}\{|\emptyset\rangle\}$.

For $k = 2$ there are two different forms of solving $m^{(j_1)} + m^{(j_2)} = j_1 + j_2 - 1$. Thus, the pair of states $|j_1, j_1\rangle \otimes |j_2, j_2 - 1\rangle$ and $|j_1, j_1 - 1\rangle \otimes |j_2, j_2\rangle$ belong to the same weight $j_1 + j_2 - 1$ in $\mathcal{H}_{(j_1, j_2)}$. One of them has been already included in $\mathcal{H}_{j_1+j_2}$, so that this does not belong to \mathcal{H}_R . The remaining vector is the extremal state of an irreducible representation $\Delta_{j_1+j_2-1}$ with $|j, j-1\rangle = |j_1, j_1\rangle \otimes |j_2, j_2 - 1\rangle$ for $j_1 \geq j_2$, or $|j, j-1\rangle = |j_1, j_1 - 1\rangle \otimes |j_2, j_2\rangle$ for $j_2 \geq j_1$, and

$$\mathcal{H}_{j_1+j_2-1} = \text{Sp}\{|j, j-1\rangle, J_-^{(j_1+j_2-1)}|j, j-1\rangle, \dots, J_-^{2(j_1+j_2-1)}|j, j-1\rangle\}.$$

Hence, the vector space (101) is rewritten as $\mathcal{H}_{(j_1, j_2)} = \mathcal{H}_{j_1+j_2} \oplus \mathcal{H}_{j_1+j_2-1} \oplus \mathcal{H}_{R'}$, with $\mathcal{H}_{R'} \cap \mathcal{H}_{j_1+j_2} \oplus \mathcal{H}_{j_1+j_2-1} = \text{Sp}\{|\emptyset\rangle\}$. The procedure can be repeated at will by noticing that each irreducible representation Δ_j is $2j + 1$ -dimensional with $j = j_1 + j_2, j_1 + j_2 - 1, \dots, |j_1 - j_2| - 1, |j_1 - j_2|$. One then arrives at the expression

$$\mathcal{H}_{(j_1, j_2)} = \mathcal{H}_{j_1+j_2} \oplus \mathcal{H}_{j_1+j_2-1} \oplus \dots \oplus \mathcal{H}_{|j_1-j_2|-1} \oplus \mathcal{H}_{|j_1-j_2|} \equiv \tilde{\mathcal{H}}_{(j_1, j_2)}$$

The k -th term in the above direct sum has the dimension

$$d_k = 2(j_1 + j_2 + 1 - k) + 1 = 2(j_1 + j_2) + 3 - 2k = n_1 + n_2 + 1 - 2k. \quad (115)$$

The following property shows that the dimension d_k of the representation space \mathcal{H}_k is reduced in two units as the value of $j = j_1 + j_2 + 1 - k$ increases in one unit. This will be useful in the sequel

$$d_k = d_{k-1} - 2, \quad k \geq 2. \quad (116)$$

Then, as expected, for the dimension of the entire space we have

$$\text{Dim}(\tilde{\mathcal{H}}_{(j_1, j_2)}) = \begin{cases} \sum_{k=1}^{2j_2+1} d_k = (2j_2 + 1)(2j_1 + 1) = n_2 n_1, & j_1 \geq j_2 \\ \sum_{k=1}^{2j_1+1} d_k = (2j_1 + 1)(2j_2 + 1) = n_1 n_2, & j_2 \geq j_1 \end{cases}$$

Let $j_0 = \min\{j_1, j_2\}$, then $n_0 = 2j_0 + 1 = \min\{n_1, n_2\}$, and

$$\tilde{\mathcal{H}}_{(j_1, j_2)} = \underbrace{\mathcal{H}_{j_1+j_2} \oplus \mathcal{H}_{j_1+j_2-1} \oplus \cdots \oplus \mathcal{H}_{|j_1-j_2|-1} \oplus \mathcal{H}_{|j_1-j_2|}}_{n_0 \text{ terms}}. \quad (117)$$

We now look for the operators Δ_j leaving invariant the subspaces \mathcal{H}_j in (117), with $j_1 + j_2 \geq j \geq |j_1 - j_2|$. That is, we want to construct the solution to the Clebsch-Gordan problem $\Delta^{(j_1, j_2)} \rightarrow \tilde{\Delta}^{(j_1, j_2)}$, with $\tilde{\Delta}^{(j_1, j_2)}$ the direct sum operator

$$\tilde{\Delta}^{(j_1, j_2)} = \Delta_{j_1+j_2} \oplus \Delta_{j_1+j_2-1} \oplus \cdots \oplus \underbrace{\Delta_{j_1+j_2+1-k}}_{k\text{-th term}} \oplus \cdots \oplus \Delta_{|j_1-j_2|-1} \oplus \Delta_{|j_1-j_2|}. \quad (118)$$

The first k terms in the direct sum (118) integrate a square matrix of order

$$z_k = \sum_{\ell=1}^k d_\ell = k(d_k + k - 1), \quad k = 1, 2, \dots, 2j_2 + 1. \quad (119)$$

Therefore, $\Delta_{j_1+j_2+1-k}$ in (118) is a square matrix of order d_k , the first element of which is at the $(z_{k-1} + 1, z_{k-1} + 1)$ entrance of $\tilde{\Delta}^{(j_1, j_2)}$ with

$$z_{k-1} = (k-1)(d_k + k), \quad z_0 := 0. \quad (120)$$

In this form, the basis elements $\tilde{J}_\alpha^{(j_1, j_2)}$, $\alpha = 3, \pm$, should read

$$\tilde{J}_\alpha^{(j_1, j_2)} = J_\alpha^{(j_1+j_2)} \oplus \cdots \oplus \underbrace{J_\alpha^{(j_1+j_2+1-k)}}_{k\text{-th term}} \oplus \cdots \oplus J_\alpha^{(|j_1-j_2|)}, \quad J_\alpha^{(0)} := 0. \quad (121)$$

For $\alpha = 3$, the Hubbard representation of the k -th term in (121) is given by

$$J_3^{(j_1+j_2+1-k)} = \sum_{p=1}^{d_k} \left(m_k^{(j_1)} + m_p^{(j_2)} \right) X_{n_1 n_2}^{z_{k-1}+p, z_{k-1}+p}, \quad z_0 = 0,$$

where we have used (103). Hence, the entire operator reads

$$\tilde{J}_3^{(j_1, j_2)} = \sum_{k=1}^{n_0} \sum_{p=1}^{d_k} \left(m_k^{(j_1)} + m_p^{(j_2)} \right) X_{n_1 n_2}^{z_{k-1}+p, z_{k-1}+p}, \quad n_0 = \min\{n_1, n_2\}. \quad (122)$$

In a similar form we get

$$\tilde{J}_+^{(j_1, j_2)} = \sum_{k=1}^{n_0} \sum_{p=1}^{d_k-1} c_{k,p}^{(j_1, j_2)} X_{n_1 n_2}^{z_{k-1}+p, z_{k-1}+p+1}, \quad c_{k,p}^{(j_1, j_2)} = \sqrt{p[2(j_1 + j_2 - k) + 3 - p]}. \quad (123)$$

Let us give a pair of examples. The following results can be compared with those we have reported in Sections 6.1.1 and 6.1.3.

6.2.1 Weights $j_1 = j_2 = 1/2$

$$\tilde{J}_3^{(\frac{1}{2}, \frac{1}{2})} = X_4^{1,1} - X_4^{3,3} = \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array} \right) = \left(\begin{array}{c|c} J_3^{(1)} & 0_{3 \times 1} \\ \hline 0_{1 \times 3} & 0 \end{array} \right) = J_3^{(\frac{1}{2}+\frac{1}{2})} \oplus J_3^{(|\frac{1}{2}-\frac{1}{2}|)},$$

$$\tilde{J}_+^{(\frac{1}{2}, \frac{1}{2})} = \sum_{p=1}^2 c_{1,p}^{(\frac{1}{2}, \frac{1}{2})} X_4^{p,p+1} = \left(\begin{array}{ccc|c} 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array} \right) \equiv \left(\begin{array}{c|c} J_+^{(1)} & 0_{3 \times 1} \\ \hline 0_{1 \times 3} & 0 \end{array} \right) = J_+^{(\frac{1}{2}+\frac{1}{2})} \oplus J_+^{(|\frac{1}{2}-\frac{1}{2}|)}.$$

6.2.2 Weights $j_1 = 1$ and $j_2 = \frac{1}{2}$

$$\begin{aligned} \tilde{J}_3^{(1, \frac{1}{2})} &= \sum_{p=1}^4 \left(\frac{5}{2} - p \right) X_6^{p,p} + \sum_{p=1}^2 \left(\frac{3}{2} - p \right) X_6^{4+p, 4+p} = \left(\begin{array}{cccc|cc} \frac{3}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{3}{2} & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} \end{array} \right) \\ &= \left(\begin{array}{c|c} J_3^{(\frac{3}{2})} & 0_{4 \times 2} \\ \hline 0_{2 \times 4} & J_3^{(\frac{1}{2})} \end{array} \right) = J_3^{(1+\frac{1}{2})} \oplus J_3^{(|1-\frac{1}{2}|)} = J_3^{(\frac{1}{2}+1)} \oplus J_3^{(|\frac{1}{2}-1|)} = \tilde{J}_3^{(\frac{1}{2}, 1)}, \end{aligned}$$

$$\begin{aligned}
\tilde{J}_+^{(1, \frac{1}{2})} &= \sum_{p=1}^3 c_{1,p}^{(1, \frac{1}{2})} X_6^{p,p+1} + c_{2,1}^{(1, \frac{1}{2})} X_6^{5,6} = \left(\begin{array}{cccc|cc} 0 & \sqrt{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right) \\
&= \left(\begin{array}{c|c} J_+^{(\frac{3}{2})} & 0_{3 \times 2} \\ \hline 0_{2 \times 3} & J_+^{(\frac{1}{2})} \end{array} \right) = J_+^{(1+\frac{1}{2})} \oplus J_+^{(|1-\frac{1}{2}|)} = J_+^{(\frac{1}{2}+1)} \oplus J_+^{(|\frac{1}{2}-1|)} = \tilde{J}_+^{(\frac{1}{2}, 1)}.
\end{aligned}$$

7 Clebsch-Gordan decomposition of $SU(2) \times SU(2)$

Let us consider the transformation matrix

$$S = \sum_{k,q=1}^{n_1 n_2} S_{k,q} X_{n_1 n_2}^{k,q} \quad (124)$$

From (28) and (110) we obtain

$$J_3^{(j_1, j_2)} S = \sum_{p,q=1}^{n_1 n_2} \left(m_{p'}^{(j_1)} + m_{p+n_2-n_2 p'}^{(j_2)} S_{p,q} \right) X_{n_1 n_2}^{p,q}, \quad p' = \lceil \frac{p}{n_2} \rceil. \quad (125)$$

In similar form, equation (122) leads to

$$S \tilde{J}_3^{(j_1, j_2)} = \sum_{t=1}^{n_1 n_2} \sum_{k=1}^{n_0} \sum_{r=1}^{d_k} S_{t, z_{k-1}+r} \left(m_k^{(j_1)} + m_r^{(j_2)} \right) X_{n_1 n_2}^{t, z_{k-1}+r}.$$

The (p, q) -entrance of this last matrix is then given by

$$\left[S \tilde{J}_3^{(j_1, j_2)} \right]_{p,q} = \sum_{k=1}^{n_0} \sum_{r=1}^{d_k} S_{p, z_{k-1}+r} \left(m_k^{(j_1)} + m_r^{(j_2)} \right) \delta_{z_{k-1}+r, q}, \quad (126)$$

where we have used (33). Given q , the double sum in (126) is reduced to a single term for the labels $k_0 \in \{1, 2, \dots, n_0\}$ and $r_0 \in \{1, 2, \dots, d_{k_0}\}$ such that

$$z_{k_0-1} + r_0 = q. \quad (127)$$

Then, the equality $J_3^{(j_1, j_2)} S = S \tilde{J}_3^{(j_1, j_2)}$ holds whenever that

$$\left(m_{p'}^{(j_1)} + m_{p+n_2-n_2 p'}^{(j_2)} - m_{k_0}^{(j_1)} - m_{r_0}^{(j_2)} \right) S_{p,q} = 0. \quad (128)$$

On the other hand, the matrix elements of $J_+^{(j_1, j_2)} S$ are obtained from (111) to read

$$\left[J_+^{(j_1, j_2)} S \right]_{p, \ell} = c_{p'}^{(j_1)} S_{p+n_2, \ell} + c_{p+n_2-n_2 p'}^{(j_2)} S_{p+1, \ell}, \quad p' = \left[\frac{p}{n_2} \right]. \quad (129)$$

Now, departing from (123) one arrives at the matrix elements

$$\left[S \tilde{J}_+^{(j_1, j_2)} \right]_{p, \ell} = \sum_{k=1}^{n_0} \sum_{r=1}^{d_k-1} S_{p, z_{k-1}+r} c_{k, r}^{(j_1, j_2)} \delta_{z_{k-1}+r+1, \ell}.$$

Given ℓ , the double sum in the latter equation reduces to a single term for $k_* \in \{1, 2, \dots, n_0\}$ and $r_* \in \{1, 2, \dots, d_{k_*}-1\}$ such that $z_{k_*-1} + r_* + 1 = \ell$. Let us take $\ell = q + 1$, then this last condition is reduced to (127) with $k_* = k_0$ and $r_* = r_0$. Therefore

$$\left[S \tilde{J}_+^{(j_1, j_2)} \right]_{p, q+1} = S_{p, q} c_{k_0, r_0}^{(j_1, j_2)}, \quad r_0 \in \{1, 2, \dots, d_{k_0}-1\}. \quad (130)$$

Using this last result, and (129) with $\ell = q + 1$, one realizes that $J_+^{(j_1, j_2)} S = S \tilde{J}_+^{(j_1, j_2)}$ is fulfilled if

$$c_{p'}^{(j_1)} S_{p+n_2, q+1} + c_{p+n_2-n_2 p'}^{(j_2)} S_{p+1, q+1} = S_{p, q} c_{k_0, r_0}^{(j_1, j_2)}, \quad r_0 \in \{1, 2, \dots, d_{k_0}-1\}. \quad (131)$$

The similar procedure shows that the elements of $J_-^{(j_1, j_2)} S = S \tilde{J}_-^{(j_1, j_2)}$ are conditioned to

$$c_{(p-n_2)'}^{(j_1)} S_{p-n_2, q} + c_{p-1+n_2-n_2(p-1)'}^{(j_2)} S_{p-1, q} = S_{p, q+1} c_{k_0, r_0}^{(j_1, j_2)}, \quad r_0 \in \{1, 2, \dots, d_{k_0}-1\}. \quad (132)$$

Now, we use Lemma A3 of the appendix and make the change

$$p = \alpha n_0 + \beta, \quad \alpha = 0, 1, \dots, n_1 + n_2 - n_0 - 1, \quad \beta = 1, 2, \dots, n_0, \quad (133)$$

to rewrite equation (128) as

$$\left(m_{\alpha+1}^{(j_1)} + m_{\beta}^{(j_2)} - m_{k_0}^{(j_1)} - m_{r_0}^{(j_2)} \right) S_{\alpha n_2 + \beta, q} = (k_0 + r_0 - \alpha - \beta - 1) S_{\alpha n_2 + \beta, z_{k_0-1} + r_0} = 0,$$

where we have used (104) and (127). It is convenient to introduce the shortcut notation

$$S_{p, q} = S_{\alpha n_0 + \beta, z_{k_0-1} + r_0} = S(\alpha, \beta; k_0, r_0) = S_{\alpha, \beta}^{k_0, r_0}, \quad (134)$$

so that the latter expression reads in a simpler form

$$(k_0 + r_0 - \alpha - \beta - 1) S_{\alpha, \beta}^{k_0, r_0} = 0. \quad (135)$$

Remark that given p and q in (134), equation (135) holds for all the values of k_0 and r_0 fulfilling (127), as well as all the values of α and β solving (133). Thus, for another set of labels \tilde{k}_0, \tilde{r}_0 , and $\tilde{\alpha}, \tilde{\beta}$, fulfilling respectively (127) and (133), we get

$$(\tilde{k}_0 + \tilde{r}_0 - \tilde{\alpha} - \tilde{\beta} - 1) S_{\tilde{\alpha}, \tilde{\beta}}^{\tilde{k}_0, \tilde{r}_0} = 0.$$

This last property leads to a further simplification in the notation since k_0 and r_0 can be written without the subindex “0”, whenever they satisfy equation (127). In this context, the nontrivial matrix elements $S_{\alpha,\beta}^{k,r}$ are now identified by using (134). That is, the roots of the equation

$$k + r - \alpha - \beta - 1 = 0, \quad (136)$$

with k , r , and α , β , fulfilling (127) and (133) respectively, are the labels of the matrix elements $S_{\alpha,\beta}^{k,r} = S_{p,q}$ that can be different from zero. Using the same notation, eqs. (131) and (132) are rewritten as

$$c_{\alpha+1}^{(j_1)} S_{\alpha+1,\beta}^{k,r+1} + c_{\beta}^{(j_2)} S_{\alpha,\beta+1}^{k,r+1} = c_{k,r}^{(j_1,j_2)} S_{\alpha,\beta}^{k,r}, \quad c_{\alpha}^{(j_1)} S_{\alpha-1,\beta}^{k,r} + c_{\beta-1}^{(j_2)} S_{\alpha,\beta-1}^{k,r} = c_{k,r}^{(j_1,j_2)} S_{\alpha,\beta}^{k,r+1} \quad (137)$$

with $r \in \{1, \dots, d_k - 1\}$. To recover the conventional expression for the recurrence relations (137) we use (104) and (123), so that the equations to solve are given by

$$\sqrt{(\alpha+1)(2j_1-\alpha)} S_{\alpha+1,\beta}^{k,r+1} + \sqrt{\beta(2j_2-\beta+1)} S_{\alpha,\beta+1}^{k,r+1} = \sqrt{r(2j-2k-r+3)} S_{\alpha,\beta}^{k,r}, \quad (138)$$

and

$$\sqrt{\alpha(2j_1-\alpha+1)} S_{\alpha-1,\beta}^{k,r} + \sqrt{(\beta-1)(2j_2-\beta+2)} S_{\alpha,\beta-1}^{k,r} = \sqrt{r(2j-2k-r+3)} S_{\alpha,\beta}^{k,r+1}, \quad (139)$$

where $j = j_1 + j_2$.

7.1 Transformation into the highest dimension invariant subspace.

Let us rewrite (138) as

$$\sqrt{\frac{(\alpha+1)!(2j_1-\alpha)!}{\alpha!(2j_1-\alpha-1)!}} S_{\alpha+1,\beta}^{k,r+1} + \sqrt{\frac{\beta!(2j_2-\beta+1)!}{(\beta-1)!(2j_2-\beta)!}} S_{\alpha,\beta+1}^{k,r+1} = \sqrt{\frac{r!(2j-2k-r+3)!}{(r-1)!(2j-2k-r+2)!}} S_{\alpha,\beta}^{k,r}$$

It is convenient to take $\tilde{\alpha} = \alpha + 1$, $\tilde{\beta} = \beta + 1$, and $\tilde{r} = r + 1$ to write

$$\sqrt{\frac{\tilde{\alpha}!(2j_1-\tilde{\alpha}+1)!}{\alpha!(2j_1-\alpha-1)!}} S_{\tilde{\alpha},\tilde{\beta}}^{k,\tilde{r}} + \sqrt{\frac{(\tilde{\beta}-1)!(2j_2-\tilde{\beta}+2)!}{(\beta-1)!(2j_2-\beta)!}} S_{\alpha,\tilde{\beta}}^{k,\tilde{r}} = \sqrt{\frac{(\tilde{r}-1)!(2j-2k-\tilde{r}+4)!}{(r-1)!(2j-2k-r+2)!}} S_{\alpha,\beta}^{k,r}$$

Now, we multiply this last equation by

$$\sqrt{\frac{\alpha!(2j_1-\alpha-1)!(\beta-1)!(2j_2-\beta)!}{(\tilde{r}-1)!(2j-2k-\tilde{r}+4)!}}$$

to get

$$\begin{aligned} & \sqrt{\frac{2j_1-\tilde{\alpha}+1}{(2j_2-\beta+1)(2j-2k-\tilde{r}+4)}} \sqrt{\frac{\tilde{\alpha}!(2j_1-\tilde{\alpha})!(\beta-1)!(2j_2-\beta+1)!}{(\tilde{r}-1)!(2j-2k-\tilde{r}+3)!}} S_{\tilde{\alpha},\tilde{\beta}}^{k,\tilde{r}} \\ & + \sqrt{\frac{2j_2-\tilde{\beta}+2}{(2j_1-\alpha)(2j-2k-\tilde{r}+4)}} \sqrt{\frac{\alpha!(2j_1-\alpha)!(\tilde{\beta}-1)!(2j_2-\tilde{\beta}+1)!}{(\tilde{r}-1)!(2j-2k-\tilde{r}+3)!}} S_{\alpha,\tilde{\beta}}^{k,\tilde{r}} \\ & = \sqrt{\frac{2j-2k-r+3}{(2j_1-\alpha)(2j_2-\beta+1)}} \sqrt{\frac{\alpha!(2j_1-\alpha)!(\beta-1)!(2j_2-\beta+1)!}{(r-1)!(2j-2k-r+3)!}} S_{\alpha,\beta}^{k,r} \end{aligned}$$

Thereby, we can take

$$S_{\alpha,\beta}^{k,r} = \text{const.} \times \sqrt{\frac{(r-1)!(2j-2k-r+3)!}{\alpha!(2j_1-\alpha)!(\beta-1)!(2j_2-\beta+1)!}}, \quad k+r = \alpha+\beta+1, \quad (140)$$

to arrive at the equation

$$\sqrt{\frac{2j_1-\tilde{\alpha}+1}{(2j_2-\beta+1)(2j-2k-\tilde{r}+4)}} + \sqrt{\frac{2j_2-\tilde{\beta}+2}{(2j_1-\alpha)(2j-2k-\tilde{r}+4)}} = \sqrt{\frac{2j-2k-r+3}{(2j_1-\alpha)(2j_2-\beta+1)}}.$$

After multiplying by the square-root of $(2j-2k-r+3)(2j_1-\alpha)(2j_2-\beta+1)$ one gets

$$k+r = \alpha+\beta+1 + (k-1).$$

We realize that condition (136) is fulfilled whenever $k=1$. Then the equation (140) reduces to

$$S_{\alpha,\beta}^{1,r} = \text{const.} \times \sqrt{\frac{(r-1)!(2j-r+1)!}{\alpha!(2j_1-\alpha)!(\beta-1)!(2j_2-\beta+1)!}}, \quad r = \alpha+\beta. \quad (141)$$

To fix the constant in (141) let us complete the binomial coefficients in the radicand. Thus, we take $\text{const.} = \sqrt{(2j_1)!(2j_2)!/(2j)!}$ so that

$$S_{\alpha,\beta}^{1,r} = \left[\frac{\binom{2j_1}{\alpha} \binom{2j_2}{\beta-1}}{\binom{2j}{r-1}} \right]^{1/2}, \quad r = \alpha+\beta, \quad (142)$$

with

$$\binom{n}{m} = \frac{n!}{(n-m)!m!}$$

the binomial coefficient. Finally, it is a matter of substitution to verify that (142) is also a root of (139) for $k=1$. Then, the matrix elements $S_{\alpha,\beta}^{1,r}$ transform the representation of $J_{\alpha}^{(j_1,j_2)}$, $\alpha = \pm, z$, from the appropriate sectors of $\mathcal{H}_{(j_1,j_2)}$ into the first invariant subspace $\mathcal{H}_{j_1+j_2}$ of the Clebsch-Gordan decomposition (117-118). Moreover, the dimension $d_1 = 2j+1$ of $\mathcal{H}_{j_1+j_2}$ is the highest of the dimensions of all the invariant subspaces \mathcal{H}_j , $j_1+j_2 \geq j \geq |j_1-j_2|$, since $d_k > d_{k+1}$ implies $d_1 > d_2 > \dots > d_{n_0}$ (see eqs. 115 and 116). Next, we are going to derive the expressions for the matrix elements $S_{\alpha,\beta}^{k,r}$ involving the invariant subspaces of dimension lower than d_1 .

7.2 Transformation into invariant subspaces of lower dimension.

In this section we derive the matrix elements associated to $k \geq 2$. Let us change first $\alpha \rightarrow \alpha+1$, and then $\beta \rightarrow \beta+1$ in (139) to get the pair of equations

$$\sqrt{(\alpha+1)(2j_1-\alpha)} S_{\alpha,\beta}^{k,r} + \sqrt{(\beta-1)(2j_2-\beta+2)} S_{\alpha+1,\beta-1}^{k,r} = \sqrt{r(2j-2k-r+3)} S_{\alpha+1,\beta}^{k,r+1},$$

$$\sqrt{\alpha(2j_1-\alpha+1)} S_{\alpha-1,\beta+1}^{k,r} + \sqrt{\beta(2j_2-\beta+1)} S_{\alpha,\beta}^{k,r} = \sqrt{r(2j-2k-r+3)} S_{\alpha,\beta+1}^{k,r+1}.$$

The substitution of this system in (138) leads to the recurrence relation,

$$\begin{aligned} & \sqrt{(\alpha+1)(\beta-1)(2j_1-\alpha)(2j_2-\beta+2)} S_{\alpha+1,\beta}^{k,r} \\ &= \sqrt{\alpha\beta(2j_1-\alpha+1)(2j_2-\beta+1)} S_{\alpha-1,\beta+1}^{k,r} \\ &+ [\beta(2j_2-\beta+1) + (\alpha+1)(2j_1-\alpha) - r(2j-2k-r+3)] S_{\alpha,\beta}^{k,r}, \end{aligned} \quad (143)$$

where $k+r = \alpha + \beta + 1$. To avoid square-roots in the coefficients of (143) we make also the change

$$S_{\alpha,\beta}^{k,r} = [\alpha!(\beta)_{\overline{\alpha}}(2j_1)_{\underline{\alpha}}(2j_2-\beta+1)_{\underline{\alpha}}]^{-1/2} S_{0,k+r-1}^{k,r} E_{\alpha,\beta}^{k,r}. \quad (144)$$

Here, $S_{0,k+r-1}^{k,r}$ and $E_{\alpha,\beta}^{k,r}$ are to be determined while the Pochhammer symbols

$$(x)_{\underline{n}} = x(x-1)\cdots(x-n+1) \quad \text{and} \quad (x)_{\overline{n}} = x(x+1)\cdots(x+n-1) \quad (145)$$

respectively represent the falling and rising factorials with

$$(x)_{\overline{0}} = (x)_{\underline{0}} = 1, \quad (x)_{\overline{n}} = (x+n-1)_{\underline{n}}, \quad (x)_{\underline{n}} = (x-n+1)_{\overline{n}}. \quad (146)$$

Notice that $\alpha = 0$ in (144) leads to $\beta = k+r-1$, and necessarily $E_{0,k+r-1}^{k,r} = 1$. After introducing (144) in (143) one arrives at the recurrence relation obeyed by $E_{\alpha,\beta}^{k,r}$ in terms of the α -parameter:

$$\begin{aligned} E_{\alpha+1,k+r-\alpha-2}^{k,r} &= -\alpha(k+r-\alpha-1)(2j_2-k-r+\alpha+2)(2j_1-\alpha+1)E_{\alpha-1,k+r-\alpha}^{k,r} \\ &+ [(k+r-\alpha-1)(2j_2-k-r+\alpha+2) + (\alpha+1)(2j_1-\alpha) - r(2j-2k-r+3)]E_{\alpha,\beta}^{k,r}, \end{aligned} \quad (147)$$

with $\beta = k+r-\alpha-1$. In the solving of (147) we take $r = 1$ and proceed by induction on α . The lowest value $\alpha = 0$ gives rise to the expression

$$E_{1,k-1}^{k,1} = -(k-1)(2j_2-k+2) = -(k-1)_{\overline{1}}(2j_2-(k-1)+1)_{\underline{1}}. \quad (148)$$

For $\alpha = 1$ one gets

$$E_{2,k-2}^{k,1} = (k-2)(k-1)(2j_2-k+3)(2j_2-k+2) = (-1)^2(k-2)_{\overline{2}}(2j_2-(k-2)+1)_{\underline{2}}. \quad (149)$$

In general, for $\alpha = \ell$,

$$E_{\ell,k-\ell}^{k,1} = (-1)^\ell(k-\ell)_{\overline{\ell}}(2j_2-(k-\ell)+1)_{\underline{\ell}}. \quad (150)$$

Remark that $\ell = k$ produces $E_{k,0}^{k,1} = 0$, henceforth $\ell \leq k-1$. On the other hand, allowing $\ell = 0$ in (150) we get $E_{0,k}^{k,1} = 1$, which is consistent with the constraint indicated after Eq. (144). Thus, making $k-\ell = \beta$ and $\ell = \alpha$ with $0 \leq \ell \leq k-1$, equation (150) reads as

$$E_{\alpha,\beta}^{k,1} = (-1)^\alpha(\beta)_{\overline{\alpha}}(2j_2-\beta+1)_{\underline{\alpha}}, \quad 0 \leq \alpha \leq k-1, \quad 1 \leq \beta \leq k. \quad (151)$$

The substitution of this last result in (144) gives the expression of $S_{\alpha,\beta}^{k,1}$ in terms of $S_{0,k}^{k,1}$,

$$\begin{aligned} S_{\alpha,\beta}^{k,1} &= (-1)^\alpha \left[\frac{(\beta)_{\overline{\alpha}}}{\alpha!} \frac{(2j_2 - \beta + 1)_{\underline{\alpha}}}{(2j_1)_{\underline{\alpha}}} \right]^{1/2} S_{0,k}^{k,1} \\ &= (-1)^\alpha \left[\binom{k-1}{\alpha} \frac{(2j_2 - k + 2)_{\overline{\alpha}}}{(2j_1 - \alpha + 1)_{\overline{\alpha}}} \right]^{1/2} S_{0,k}^{k,1}, \end{aligned} \quad (152)$$

where we have used (146). Since S is unitary, we can fix the value of $S_{0,k}^{k,1}$ as follows

$$\begin{aligned} 1 = \sum_{\alpha=0}^{k-1} \left(S_{\alpha,\beta}^{k,1} \right)^2 &= \left(S_{0,k}^{k,1} \right)^2 \left[1 + \binom{k-1}{1} \frac{(2j_2 - k + 2)_{\overline{1}}}{(2j_1)_{\overline{1}}} + \cdots + \binom{k-1}{k-1} \frac{(2j_2 - k + 2)_{\overline{k-1}}}{(2j_1 - k + 2)_{\overline{k-1}}} \right] \\ &= \frac{\left(S_{0,k}^{k,1} \right)^2}{(2j_1 - k + 2)_{\overline{k-1}}} \sum_{\alpha=0}^{k-1} \binom{k-1}{\alpha} (2j_1 - k + 2)_{\overline{\alpha}} (2j_1 - k + 2)_{\overline{k-1-\alpha}}. \end{aligned}$$

Using the addition formula Lemma A4

$$(a + b)_{\overline{n}} = \sum_{s=0}^n \binom{n}{s} (a)_{\overline{s}} (b)_{\overline{n-s}} \quad (153)$$

we finally get the roots

$$S_{0,k}^{k,1} = \pm \sqrt{\frac{(2j_1 - k + 2)_{\overline{k-1}}}{(2j - 2k + 4)_{\overline{k-1}}}} = \pm \sqrt{\frac{(2j_1)_{\overline{k-1}}}{(2j - k + 2)_{\overline{k-1}}}}. \quad (154)$$

As a convention, hereafter we take the positive expression in (154) as the definition of the matrix elements $S_{0,k}^{k,1}$. Therefore, (152) becomes

$$S_{\alpha,\beta}^{k,1} = (-1)^\alpha \left[\frac{(\beta)_{\overline{\alpha}}}{\alpha!} \frac{(2j_2 - \beta + 1)_{\underline{\alpha}} (2j_1 - \alpha)_{\overline{k-1}}}{(2j - k + 2)_{\overline{k-1}}} \right]^{1/2}. \quad (155)$$

To construct the remanent matrix elements we now use the recurrence relation (139),

$$S_{\alpha,\beta}^{k,r+1} = \sqrt{\frac{\alpha(2j_1 - \alpha + 1)}{r(2j - 2k + 3)}} S_{\alpha-1,\beta}^{k,r} + \sqrt{\frac{(\beta - 1)(2j_2 - \beta + 2)}{r(2j - 2k - r + 3)}} S_{\alpha,\beta-1}^{k,1}.$$

For $r = 1$, the straightforward calculation produces

$$S_{\alpha,\beta}^{k,2} = (-1)^\alpha F_{\alpha,\beta}^{k,2} \Theta_{\alpha-1,\beta}^{k,1}, \quad (156)$$

with

$$\Theta_{\alpha-1,\beta}^{k,1} = \left[\frac{(\beta)_{\overline{\alpha-1}} (2j_2 - \beta + 1)_{\underline{\alpha-1}} (2j_1 + \beta - k)_{\overline{k-1}}}{1! (k - \beta)! (2j - k + 2)_{\overline{k-1}} (2j - 2k + 2)_{\underline{1}}} \right]^{1/2}, \quad (157)$$

and

$$\begin{aligned}
F_{\alpha,\beta}^{k,2} &= (\beta - 1)(2j_2 - \beta + 2) - \alpha(2j_1 - \alpha + 1) \\
&= [(\beta - 1)_{\overline{1}}(2j_2 - \beta + 2)_{\overline{1}}] {}_3F_2 \left[\begin{matrix} -1, -\alpha, 2j_1 - \alpha + 1 \\ \beta - 1, -2j_2 + \beta - 2 \end{matrix} \right]. \tag{158}
\end{aligned}$$

To derive (158) we have used Lemma A5 of the appendix with ${}_3F_2$ is the generalized hypergeometric function

$${}_3F_2(a, b, c; d, e; z) \equiv {}_3F_2 \left[\begin{matrix} a, b, c; z \\ d, e \end{matrix} \right] = \sum_{s=0}^{+\infty} \frac{(a)_{\overline{s}}(b)_{\overline{s}}(c)_{\overline{s}}}{(d)_{\overline{s}}(e)_{\overline{s}}} \frac{z^s}{s!}. \tag{159}$$

Here we are adopting the convention ${}_3F_2(a, b, c; d, e) \equiv {}_3F_2(a, b, c; d, e; 1)$. Now we take $r = 2$ to arrive at

$$S_{\alpha,\beta}^{k,3} = (-1)^\alpha F_{\alpha,\beta}^{k,3} \Theta_{\alpha-2,\beta}^{k,2}. \tag{160}$$

The expression for $\Theta_{\alpha-2,\beta}^{k,2}$ can be obtained from $\Theta_{\alpha-1,\beta}^{k,1}$ in (157) after the change $1 \rightarrow 2$. For the first factor in (160) we have

$$\begin{aligned}
F_{\alpha,\beta}^{k,3} &= (\beta - 1)(2j_2 - \beta + 2)F_{\alpha,\beta-1}^{k,2} - \alpha(2j_1 - \alpha + 1)F_{\alpha-1,\beta}^{k,2} \\
&= \sum_{s=0}^2 (-1)^s \binom{2}{s} (\alpha)_{\overline{s}} (\beta - 1)_{\underline{2-s}} (2j_1 - \alpha + 1)_{\overline{s}} (2j_2 - \beta + 2)_{\overline{2-s}} \\
&= [(\beta - 2)_{\overline{2}}(2j_2 - \beta + 2)_{\overline{2}}] {}_3F_2 \left[\begin{matrix} -2, -\alpha, 2j_1 - \alpha + 1 \\ \beta - 2, -2j_2 + \beta - 3 \end{matrix} \right]. \tag{161}
\end{aligned}$$

In general, one can apply induction on r to verify that the roots of the system (138-139) for $k \geq 1$ are given by

$$S_{\alpha,\beta}^{k,r+1} = (-1)^\alpha F_{\alpha,\beta}^{k,r+1} \Theta_{\alpha-r,\beta}^{k,r}, \tag{162}$$

with $\Theta_{\alpha-r,\beta}^{k,r}$ the immediate generalization of (157),

$$\Theta_{\alpha-r,\beta}^{k,r} = \left[\frac{(\beta)_{\overline{\alpha-r}}(2j_2 - \beta + 1)_{\overline{\alpha-r}}(2j_1 + \beta - k)_{\overline{k-r}}}{r! (k - \beta)! (2j - k + 2)_{\overline{k-r}}(2j - 2k + 2)_{\overline{r}}} \right]^{1/2} \tag{163}$$

and $F_{\alpha,\beta}^{k,r+1}$ the generalization of (161), see Lemma A5 of the appendix,

$$F_{\alpha,\beta}^{k,r+1} = [(\beta - r)_{\overline{r}}(2j_2 - \beta + 2)_{\overline{r}}] {}_3F_2 \left[\begin{matrix} -r, -\alpha, 2j_1 - \alpha + 1 \\ \beta - r, -2j_2 + \beta - r - 1 \end{matrix} \right]. \tag{164}$$

To close this section we give the explicit form of the matrix S for two of the cases discussed in the previous sections. If $j_1 = j_2 = \frac{1}{2}$ one has

$$S = \left(\begin{array}{ccc|c} S_{0,1}^{1,1} & 0 & 0 & 0 \\ 0 & S_{0,2}^{1,2} & 0 & S_{0,2}^{2,1} \\ \hline 0 & S_{1,1}^{1,2} & 0 & S_{1,1}^{2,1} \\ 0 & 0 & S_{1,2}^{1,3} & 0 \end{array} \right) = \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \hline 0 & -\frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & 1 & 0 \end{array} \right),$$

while $j_1 = 1$ and $j_2 = \frac{1}{2}$ leads to

$$S = \left(\begin{array}{cccc|cc} S_{0,1}^{1,1} & 0 & 0 & 0 & 0 & 0 \\ 0 & S_{0,2}^{1,2} & 0 & 0 & S_{0,2}^{2,1} & 0 \\ \hline 0 & S_{1,1}^{1,2} & 0 & 0 & S_{1,1}^{2,1} & 0 \\ 0 & 0 & S_{0,2}^{1,3} & 0 & 0 & S_{1,2}^{2,2} \\ \hline 0 & 0 & S_{2,1}^{1,3} & 0 & 0 & S_{2,1}^{2,2} \\ 0 & 0 & 0 & S_{2,2}^{1,4} & 0 & 0 \end{array} \right) = \left(\begin{array}{cccc|cc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1}{3}} & 0 & 0 & \sqrt{\frac{2}{3}} & 0 \\ \hline 0 & \sqrt{\frac{2}{3}} & 0 & 0 & -\sqrt{\frac{1}{3}} & 0 \\ 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & \sqrt{\frac{1}{3}} \\ \hline 0 & 0 & \sqrt{\frac{1}{3}} & 0 & 0 & -\sqrt{\frac{2}{3}} \\ 0 & 0 & 0 & 1 & 0 & 0 \end{array} \right).$$

7.3 Addition of angular momenta

Consider a bipartite system integrated by independent subsystems $\mathcal{S} = \mathcal{S}_1 + \mathcal{S}_2$. Any of the observables belonging to \mathcal{S} should be constructed in terms of the Kronecker products $A \otimes B$, with A and B observables (identities included) of \mathcal{S}_1 and \mathcal{S}_2 respectively. The product $SU(2) \times SU(2)$ defines the symmetry for the coupled system $\mathcal{S} = \mathcal{S}_1 + \mathcal{S}_2$, where the Lie group $SU(2)$ represents the symmetry of each of the subsystems \mathcal{S}_1 and \mathcal{S}_2 . That is, the component \mathcal{S}_k is characterized by the requirement that the n_k -dimensional vector space $\text{Sp}\{|e_{i_k}^{n_k}\rangle\}_{i_k=1}^{n_k}$ defines an irreducible representation of $SU(2)$ for $k = 1, 2$ (This is the situation for the 1H and ^{13}C nuclei which are both $SU(2)$ nuclear spin systems, and $^1H^{13}C$ which is a $SU(2) \times SU(2)$ system [41]). Then, the angular momenta \vec{J}_1 , \vec{J}_2 , as well as their sum $\vec{J} = \vec{J}_1 + \vec{J}_2$, are conserved. These quantities are respectively the generators of the rotations acting on the first system alone, the second one alone, and both systems simultaneously [15]. The diagonalization of $\vec{J} \cdot \vec{J}$ and $\vec{J}_z = \vec{J}_{1z} + \vec{J}_{2z}$ gives rise to the orthonormal basis vectors $|J, M\rangle$ belonging to the eigenvalues $J(J+1)$ and M respectively. The two subsystems in turn are described by a state vector which belongs to $\text{Sp}\{|j_1, m^{(j_1)}\rangle \otimes |j_2, m^{(j_2)}\rangle\}$, with $J = j_1 + j_2$ and $M = m^{(j_1)} + m^{(j_2)}$. This is therefore useful to know the coefficients of the change of basis

$$|J, M\rangle = \sum_{m^{(j_1)}, m^{(j_2)}} \langle j_1, m^{(j_1)}; j_2, m^{(j_2)} | J, M \rangle |j_1, m^{(j_1)}; j_2, m^{(j_2)}\rangle. \quad (165)$$

7.3.1 Clebsch-Gordan coefficients

Let $\{|J, M\rangle\}_{M=-J}^J$ be the eigenvectors of the operator (87) and S the unitary matrix defined in (124). Since S is unitary we may write

$$\begin{aligned} M &= \langle J, M | \tilde{J}_3^{(j_1, j_2)} | J, M \rangle = \langle J, M | S^\dagger J_3^{(j_1, j_2)} S | J, M \rangle \\ &= \langle j_1, m^{(j_1)}; j_2, m^{(j_2)} | J_3^{(j_1, j_2)} | j_1, m^{(j_1)}; j_2, m^{(j_2)} \rangle = m^{(j_1)} + m^{(j_2)}, \end{aligned}$$

where $|j_1, m^{(j_1)}; j_2, m^{(j_2)}\rangle = |j_1, m^{(j_1)}\rangle \otimes |j_2, m^{(j_2)}\rangle$ and the Corollary TM2.2 was used. Therefore, up to a global phase (fixed as 1), we must have

$$|j_1, m^{(j_1)}; j_2, m^{(j_2)}\rangle = S |J, M\rangle.$$

Hence

$$\langle J', M' | j_1, m^{(j_1)}; j_2, m^{(j_2)} \rangle = \langle J', M' | S | J, M \rangle$$

defines the Clebsch-Gordan coefficient required in (165). Thus, the entries of the (unitary) transformation matrix S are associated to the coupling coefficients of $SU(2) \otimes SU(2)$.

8 Concluding remarks

We have applied the Hubbard operators in the study of the Kronecker product of square matrices. The former represent a shorthand notation for the direct product that transforms complicated calculations involving large matrices or a large number of factors into simple relations of subscripts. Thus, the Hubbard representation is compact enough to facilitate the study of the algebra and group properties of the observables defining a multipartite quantum system, no matter the order or the number of the corresponding matrices. In particular, we have shown that the construction of permutation matrices, the identification of the corresponding permutation classes of equivalence and the construction of symmetrization operators is straightforward. All the basic properties of the Kronecker product of square matrices have been revisited in the Hubbard representation. In this framework the proofs of the corresponding theorems, lemmas and corollaries are achieved in easy form. As an immediate application we have constructed irreducible representations of $SU(2)$ by giving concrete expressions for the involved matrices in Hubbard notation. The same has been done for the product group $SU(2) \times SU(2)$. The solution of the Clebsch-Gordan decomposition of $SU(2) \times SU(2)$ by using the Hubbard representation lead to definite expressions for the Clebsch-Gordan coefficients of the addition of angular momenta in terms of the hypergeometric function ${}_3F_2$. Some connections can be found with the results already reported in [42]. In this context we like to stress that our results are in contraposition to the common affirmation that “it is not possible to give a general expression for the Clebsch-Gordan coefficients” (see e.g. [43], pp 1023). Therefore, the expressions derived in Section 7 of the present work give an alternative to obtain the Clebsch-Gordan coefficients that is different from the calculating by iteration or the checking in numerical tables. We hope our results have shed some light on the matter.

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A Appendix

Some properties of the ceiling function $\lceil \cdot \rceil$ and the floor function $\lfloor \cdot \rfloor$ used through this paper are proven. For a given real number x the ceiling function

$$\lceil x \rceil = \min\{z \in \mathbb{Z} : x \leq z\} \quad (\text{A.2})$$

yields the smallest integer greater than or equal to x . On the another hand, the floor function

$$\lfloor x \rfloor = \max\{z \in \mathbb{Z} : z \leq x\} \quad (\text{A.3})$$

gives the largest previous integer to x .

Lemma A1. For $x \in \mathbb{R}$ and $m, n \in \mathbb{N}$ it is fulfilled

$$(i) \lceil x \rceil = n \text{ if and only if } x \leq n < x + 1$$

$$(ii) \lceil x + n \rceil = \lceil x \rceil + n.$$

$$(iii) \lfloor x + n \rfloor = \lfloor x \rfloor + n.$$

$$(iv) \left\lceil \frac{x}{mn} \right\rceil = \left\lceil \frac{\lceil x/n \rceil}{m} \right\rceil.$$

$$(v) \left\lfloor \frac{n+1}{m} \right\rfloor = \left\lfloor \frac{n}{m} \right\rfloor + 1.$$

Proof.

(i) From the definition of ceiling function it is clear that

$$\lceil x \rceil = n \text{ if and only if } n - 1 < x \leq n. \quad (\text{A.4})$$

Rearranging these last inequalities we get $x \leq n < x + 1$.

(ii) By virtue of (A.4) we may write

$$\lceil x \rceil - 1 < x \leq \lceil x \rceil.$$

Then

$$\lceil x \rceil + n - 1 < x + n \leq \lceil x \rceil + n,$$

and (A.4) implies $\lceil x + n \rceil = \lceil x \rceil + n$.

(iii) Departing from

$$\lfloor x \rfloor \leq x < \lfloor x \rfloor + 1, \quad (\text{A.5})$$

one gets

$$\lfloor x \rfloor + n \leq x + n < \lfloor x \rfloor + n + 1,$$

and $\lfloor x + n \rfloor = \lfloor x \rfloor + n$.

(iv) Consider a continuous, monotonically increasing function f . We know that if $f(x)$ is an integer then x is an integer [39]. Therefore

$$\lceil f(x) \rceil = \lceil f(\lceil x \rceil) \rceil. \quad (\text{A.6})$$

Let us take the continuous and monotonically increasing function $f(x) = \frac{x}{m}$. According to the statement above, if $f(x) = k$ with $k \in \mathbb{Z}$, then $x = km$ is an integer. Hence, from equation (A.6) it follows

$$\left\lceil \frac{x}{m} \right\rceil = \left\lceil \frac{\lceil x \rceil}{m} \right\rceil,$$

Make $x \rightarrow x/n$ in the last equation the proof is completed.

(v) According to (A.4) we may write

$$\left\lceil \frac{n+1}{m} \right\rceil - 1 < \frac{n+1}{m} \leq \left\lceil \frac{n+1}{m} \right\rceil. \quad (\text{A.7})$$

From the right inequality we get

$$\frac{n}{m} \leq \left\lceil \frac{n+1}{m} \right\rceil - \frac{1}{m} < \left\lceil \frac{n+1}{m} \right\rceil.$$

Adding 1 in both sides one has

$$\frac{n}{m} + 1 < \left\lceil \frac{n+1}{m} \right\rceil + 1. \quad (\text{A.8})$$

The left inequality in (A.7) implies $\left\lceil \frac{n+1}{m} \right\rceil < \frac{n}{m} + 1 + \frac{1}{m}$, this is true if and only if

$$\left\lceil \frac{n+1}{m} \right\rceil \leq \frac{n}{m} + 1. \quad (\text{A.9})$$

Combining (A.8) and (A.9) we arrive at

$$\left\lceil \frac{n+1}{m} \right\rceil \leq \frac{n}{m} + 1 < \left\lceil \frac{n+1}{m} \right\rceil + 1.$$

From equation (A.5) we see that

$$\left\lfloor \frac{n}{m} + 1 \right\rfloor = \left\lceil \frac{n+1}{m} \right\rceil. \quad (\text{A.10})$$

Using (iii) in the left side of this last equation one gets the result we are looking for. \square

Lemma A2. Let $F(i, j, k, l)$ be a function of the indices i, j, k, l . Then

$$\sum_{i,j}^m \sum_{k,l}^n F(i, j, k, l) \delta_{n(j-1)+l}^{n(i-1)+k} = \sum_{i,j}^m \sum_{k,l}^n F(i, j, k, l) \delta_i^j \delta_k^l. \quad (\text{A.11})$$

Proof. Let us define $p = n(i-1) + k$ and $q = n(j-1) + l$. Note that $p, q = 1, 2, \dots, mn$. Thus

$$\begin{aligned}
& \sum_{i,j}^m \sum_{k,l}^n F(i, j, k, l) \delta_{n(j-1)+l}^{n(i-1)+k} \\
&= \sum_{i,j}^m \sum_{p=n(i-1)+1}^{ni} \sum_{q=n(j-1)+1}^{nj} F(i, k, p - n(i-1), q - n(j-1)) \delta_p^q \\
&= \sum_{p,q} F(p', q', p'', q'') \delta_p^q = \sum_p F(p', p', p'', p'') \\
&= \sum_{i=1}^m \sum_{p=n(i-1)+1}^{ni} F(i, i, p - n(i-1), p - n(i-1)) \\
&= \sum_{i=1}^m \sum_{k=1}^n F(i, i, k, k) = \sum_{i,j}^m \sum_{k,l}^n F(i, j, k, l) \delta_i^j \delta_k^l.
\end{aligned}$$

Where we have used Lemma A1(i). \square

Lemma A3. Let $\alpha, \beta, n_1, n_2 \in \mathbb{N}$ be such that $\alpha = 1, \dots, n_1 - 1$; $\beta = 1, \dots, n_2$, with $n_1 \geq n_2$. The ceiling function satisfies the following properties

- (i) $\left\lceil \frac{\beta}{n_2} \right\rceil = 1$.
- (ii) $p' = \alpha + 1$, where $p' = \left\lceil \frac{p}{n_2} \right\rceil$
- (iii) $(p - n_2)' = \alpha$, for $\alpha > 0$.

Proof.

- (i) For any $x \in \mathbb{R}$ we have $\lceil x \rceil = 1$ if $x \leq 1$. The proof follows by noticing that $\frac{\beta}{n_2} \leq 1$.
- (ii) Using (i) and Lemma A1(iii) one gets

$$p' = \left\lceil \frac{\alpha n_2 + \beta}{n_2} \right\rceil = \left\lceil \alpha + \frac{\beta}{n_2} \right\rceil = \alpha + \left\lceil \frac{\beta}{n_2} \right\rceil = \alpha + 1,$$

where $\beta = p - n_2 p' + n_2$.

- (iii) The proof is similar to the one of (ii). Yet,

$$(p - n_2)' = \left\lceil \frac{\alpha n_2 + \beta - n_2}{n_2} \right\rceil = \left\lceil \alpha - 1 + \frac{\beta}{n_2} \right\rceil = \alpha - 1 + 1 = \alpha. \quad \square$$

Lemma A4. Let $n, a, b \in \mathbb{N}$. We have

$$\sum_{i=0}^n \frac{(a)_{\overline{n-i}} (b)_{\overline{n}}}{(n-i)! i!} = \frac{(a+b)_{\overline{n}}}{n!}, \quad (\text{A.12})$$

where $(x)_{\overline{n}} = x(x+1) \cdots (x+n-1)$.

Proof. From the binomial expansion we have

$$(1-x)^{-a} = \sum_{j=0}^{\infty} \frac{(a)_{\overline{j}}}{j!} x^j.$$

Note

$$(1-x)^{-a}(1-x)^{-b} = \left(\sum_{l=0}^{\infty} \frac{(a)_{\overline{l}}}{l!} \right) \left(\sum_{m=0}^{\infty} \frac{(b)_{\overline{m}}}{m!} \right) = \sum_{l,m} \frac{(a)_{\overline{l}} (b)_{\overline{m}}}{l!m!} x^{l+m}$$

We make the change $i = l + m$ to get

$$(1-x)^{-a}(1-x)^{-b} = \sum_{m=0}^{\infty} \sum_{i=m}^{\infty} \frac{(a)_{\overline{i-m}} (b)_{\overline{m}}}{(i-m)! m!} x^i = \sum_{i=0}^{\infty} \sum_{m=0}^i \frac{(a)_{\overline{i-m}} (b)_{\overline{m}}}{(i-m)! m!} x^i.$$

On the other hand,

$$(1-x)^{-(a+b)} = \sum_{n=0}^{\infty} \frac{(a+b)_{\overline{n}}}{n!} x^n.$$

Comparing term by term the two last equations the proof is completed. \square

Lemma A5. The generalized hypergeometric function ${}_3F_2$ satisfies

$$(d)_{\overline{r}}(e)_{\underline{r}} {}_3F_2(-r, -b, c; d, -e) = \sum_{s=0}^r (-1)^s \binom{r}{s} (b)_{\underline{s}} (c)_{\overline{s}} (d+1)_{\underline{r-s}} (e)_{\underline{r}}, \quad (\text{A.13})$$

with $r, b, c, d, e \in \mathbb{Z}$. The right and left Pochhammer symbols are defined as $(x)_{\overline{n}} = x(x+1) \cdots (x+n-1)$ and $(x)_{\underline{n}} = x(x-1) \cdots (x-n+1)$, respectively.

Proof. Let us take $r = 1$, then

$${}_3F_2(-1, -b, c; d, -e) = \frac{1}{de} (de - bc) = \frac{1}{(d)_{\overline{1}}(e)_{\underline{1}}} \sum_{s=0}^1 (-1)^s \binom{1}{s} (b)_{\underline{s}} (c)_{\overline{s}} (d+1)_{\underline{1-s}} (e)_{\underline{1}}.$$

If now we set $r = 2$,

$$\begin{aligned} {}_3F_2(-2, -b, c; d, -e) &= 1 - \frac{2bc}{de} + \frac{b(b-1)c(c+1)}{d(d+1)e(e-1)} \\ &= \frac{1}{(d)_{\overline{2}}(e)_{\underline{2}}} \sum_{s=0}^2 (-1)^s \binom{2}{s} (b)_{\underline{s}} (c)_{\overline{s}} (d+1)_{\underline{2-s}} (e)_{\underline{2}}. \end{aligned}$$

The proof is completed by induction on r . \square

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